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Laboratory Directed Research & Development Program

Annual Report to the Department of Energy For Fiscal Year 1999

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BROOKHAVEN NATIONAL LABORATORY
BROOKHAVEN SCIENCE ASSOCIATES
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DISCLAIMER

Acknowledgments

The Laboratory Directed Research and Development (LDRD) Program is directed by Peter Paul, Deputy Director for Science & Technology, and is managed by Kevin Fox, Special Assistant to the Assistant Laboratory Director for Finance & Administration (ALDFA). Preparation of the FY 1999 report was coordinated and edited by Kevin Fox and Peter Yamin, who wish to thank D.J. Greco and Regina Paquette for their assistance in organizing, typing, and proofing the document. A special thank you is also extended to the Photography and Graphic Arts Group for their help in publishing. Of course, a very special acknowledgement is extended to all of the authors of the project annual reports and to their assistants.

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Introduction

Background: Brookhaven National Laboratory (BNL) was established in 1947 on the site of the former Army Camp Upton. Brookhaven is a multidisciplinary laboratory that carries out basic and applied research in the physical, biomedical and environmental sciences, and in selected energy technologies. It is managed by Brookhaven Science Associates, LLC, under contract with the U. S. Department of Energy. BNL's total annual budget has averaged about $407 million, and its facilities are book valued at over $3.8 billion. There are about 3,000 employees, and another 4,500 guest scientists and students who come each year to use the Laboratory's facilities and work with the staff. BNL's Relativistic Heavy Ion Collider (RHIC), which was commissioned in June 1999, will be the world's foremost facility for nuclear physics research. RHIC will create the hot, dense plasma of quarks and gluons from which particles condensed after the "Big Bang" of the early universe.

Mission and Core Competencies: Brookhaven National Laboratory's mission is to produce excellent science in a safe, environmentally benign manner with the cooperation, support, and appropriate involvement of our many communities. Brookhaven was founded as a laboratory which would provide specialized research facilities that could not be designed, built and operated at a university or industrial complex, and provides a scientific core effort for these facilities. This still remains a basic mission of the Laboratory.

Brookhaven National Laboratory has four core competencies: Research Facilities, Scientific Research, Technology Development, and Knowledge Transfer which are not independent isolated competencies. They are interrelated in a complex manner.

MAJOR CORE COMPETENCIES
RESEARCH FACILITIES Conceive, design, construct, and operate complex, leading-edge, user-oriented facilities in a safe and environmentally benign manner that is responsive to the DOE, and the needs of the users.
SCIENTIFIC RESEARCH Carry out basic and applied research in long-term programs at the frontier of science that supports DOE missions and the needs of the Laboratory's users community.
TECHNOLOGY DEVELOPMENT Develop advanced technologies that address national needs and initiate their transfer to other organizations and to the commercial sector.
KNOWLEDGE TRANSFER Disseminate technical knowledge to educate new generations of scientists and engineers, to maintain technical currency in the nation's workforce, and to encourage scientific awareness in the general public.

Research Facilities and Scientific Research have a synergistic relationship. To maintain and constantly improve a research facility, and to keep it at the cutting edge, it is essential that the Laboratory have a significant research staff of excellent stature. The staff drives the performance of the facility. Having several complementary facilities at one location, such as the National Synchrotron Light Source and the Alternating Gradient Synchrotron, allows unique research capabilities. The other two core competencies: Technology Development and Knowledge Transfer, bridge all of the research facilities and research programs.

Brookhaven's core competencies support and cut across the four central activities of the Department of Energy as defined in its Strategic Plan.

DOE Strategic Plan Activities	
SCI	**Science and Technology**
ENV	**Environmental Quality**
ENER	**Energy Security**
SEC	**National Security**

BNL plays a major role in the Science and Technology, the Environmental Quality, the Industrial Competitiveness and the Energy Resources sectors, with a smaller, but special role in the National Security arena. In order to better see the connection between the various Brookhaven activities that form the core competencies and the Department of Energy Strategic Plan activities, each BNL activity/competency is followed with the letter code describing the match in the Table 1, "Major Activity Clusters."

Summary of the LDRD Program: As one of the premier scientific laboratories of the DOE, Brookhaven must continuously foster the development of new ideas and technologies, promote the early exploration and exploitation of creative and innovative concepts, and develop new "fundable" R&D projects and programs. At Brookhaven National Laboratory one such method is through its Laboratory Directed Research and Development Program. This discretionary research and development tool is critical in maintaining the scientific excellence and long-term vitality of the Laboratory. Additionally, it is a means to stimulate the scientific community, fostering new science and technology ideas, which is a major factor in achieving and maintaining staff excellence and a means to address national needs within the overall mission of the DOE and BNL.

The Project Summaries with their accomplishments described in this report reflect the above. Aside from leading to new fundable or promising programs and producing especially noteworthy research, they have resulted in numerous publications in various professional and scientific journals and presentations at meetings and forums.

TABLE 1:
MAJOR ACTIVITY CLUSTERS

LARGE RESEARCH FACILITIES

ALTERNATING GRADIENT SYNCHROTRON
(SCI)
- Research in Particle and Nuclear Physics
- High-Intensity Frontier of Particle Physics
- World's Only High Energy Polarized Proton Source
- At Present, Nation's Only High Energy, Heavy Ion Synchrotron
- Research in Radiobiology
- Over 900 Users

RELATIVISTIC HEAVY ION COLLIDER
(SCI)
- Dedicated Colliding Beams Facility for Ultra Relativistic Collisions of Heavy Nuclei
- Highest Priority Construction Project for U.S. Nuclear Physics
- New Phases of Nuclear Matter High-Temperature Frontier
- Large and Unique High Energy Physics Potential (e.g. spin physics)
- International Community of Over 800 Scientists

NATIONAL SYNCHROTRON LIGHT SOURCE
(SCI, ENV, ENER)
- Two Storage Rings Providing Intense UV and X-ray Photon Sources
- 83 Beamlines for Research in Materials Science, Biology, Chemistry, Medical and Industrial Applications
- R&D on Free Electron Lasers and on Production and Utilization of Synchrotron Radiation
- Over 2300 Users, Including 400 Industrial Users

BIOMEDICAL FACILITIES

BROOKHAVEN CENTER FOR IMAGING AND NEUROSCIENCE
(SCI)
- Positron Emission Tomography (PET)
- Single Photon Emission Computed Tomography (SPECT)
- High-Field (4 Tesla) Magnetic Resonance Imaging (MRI)
- Used for Research in the Basic and Clinical Neuroscience (Substance Abuse; Aging; Brain Cancer; Drug Research) and the Development of New Forms of Imaging

BROOKHAVEN LINEAR ISOTOPE PRODUCTION FACILITY
(SCI)
- Production of Isotopes for Medical Purposes
- Approximately 20 Isotopes Produced for Commercial and/or Research Use

MEDICAL RADIATION FACILITY
(SCI)
- Cancer Patient Treatment: 250 patients annually

BROOKHAVEN MEDICAL RESEARCH REACTOR
(SCI)
- Neutron Capture Cancer Therapy Research

SCANNING TRANSMISSION ELECTRON MICROSCOPE
(SCI)
- Structural Biology, Molecular Masses
- Over 75 Users

PROTEIN DATA BANK
(SCI)
- World-Wide Repository for Three-Dimensional Structures of Biological Macromolecules
- 6,380 Structures on File, 350,000 Accesses/Year

GENOME SEQUENCING CENTER
(under development)
(SCI)
- Large-Scale DNA Sequencing

OTHER FACILITIES

TANDEM VAN DE GRAAFF FACILITY
(SCI, SEC, ENV, ENER)
- Injector (source) for Heavy Ions for AGS/RHIC
- Microchip Radiation Testing Facility
- Film Irradiation Plant for Track Etching Filter Membranes
- 250 Users from 45 Institutions

ACCELERATOR TEST FACILITY
(SCI, SEC)
- Advanced Acceleration Concepts and Generation of Coherent Radiation
- Short Wavelength Free-Electron Laser Research

CENTER FOR RADIATION CHEMISTRY RESEARCH
(SCI, ENER, ENV)
- Study of Rapid Chemical Reactions: Catalysis, Energy Conversion and Storage, Waste Management

NATIONAL NUCLEAR DATA CENTER
(SCI, SEC, ENV)
- Nuclear Cross-Section and Structure Data
- 1,100 Users

BOOSTER APPLICATIONS FACILITY
(under development)
(SCI)
- Proton and Heavy Ion Radiobiology
- Microelectronics Radiation Effects

SCIENTIFIC RESEARCH

HIGH ENERGY PARTICLE AND NUCLEAR PHYSICS
(SCI)
- Beyond the Standard Model
  - Rare Kaon Decays
  - Muon Anomalous Magnetic Moment
  - Exotics and Glueball Spectroscopy
  - Strange Matter
  - Solar Neutrinos
- Relativistic Heavy Ions
  - Nuclear Matter In Extreme States of Temperature and Density
  - QCP Phase Transitions: Hadrons to Quark-Gluon Plasma
  - Recreate Conditions of the Early Universe, Microseconds after the Big Bang

ADVANCED ACCELERATOR CONCEPTS
(SCI, SEC)
- Short Wavelength Accelerating Structures
- Production of Coherent Radiation Free Electron Laser
- Muon Collider
- Neutron Sources
- Interlaboratory Cooperation to Design and Build SNS

MATERIALS SCIENCES
(SCI, ENER)
- Magnetism and Superconductivity
- Surface Studies – Catalysis, Corrosion, and Adhesion
- Condensed Matter Theory: Metallic Alloys and Cooperative Phenomena
- Materials Synthesis and Characterization with Neutron and X-Ray Scattering:
- Structure and Dynamics
- Defect Structure with Positrons

CHEMICAL SCIENCES
(SCI, ENER, ENV)
- Dynamics and Energetics and Reaction Kinetics
- Thermal, Photo- and Radiation-Induced Reactions
- Catalysis and Interfacial Chemistry
- Homogeneous Catalysis with Metal Hybride Complexes
- Porphyrin Chemistry
- Electrochemistry

ENVIRONMENTAL SCIENCES
(SCI, ENV)
- Global Change
- Atmospheric Chemistry
- Marine Science
- Soil Chemistry
- Cycling of Pollutants
- Environmental Remediation

MEDICAL SCIENCE
(SCI)
- Medical Imaging: PET, SPECT, MRI, Coronary Angiography
- Nuclear Medicine
- Radionuclides, Radiopharmaceuticals, Synthesis and Applications
- Advanced Cancer Therapies: Neutron Capture, Microbeam Radiation, Proton Radiation, Photon Activation Therapy (PAT)
- Mechanisms of Oncogenesis

MOLECULAR BIOLOGY AND BIOTECHNOLOGY
(SCI)
- Genome Structure, Gene Expression, Molecular Genetics
- DNA Replication, Damage and Repair
- Structure and Function of Enzymes, Protein Engineering
- Plant Genomics, Biochemistry and Energetics

- Solution Structure, Kinetics and Interaction of Biomolecules
- Bio-Structure Determination by X-ray and Neutron Scattering
- Bio-Structure Determination and Mass Measurements by Electron Microscopy

ADVANCED SCIENTIFIC COMPUTING AND SYSTEMS ANALYSIS
(SCI, ENV, ENER)
- Risk Assessment
- Energy Modeling
- Groundwater Modeling
- Traffic Congestion Simulation
- Atmospheric Transport Modeling

TECHNOLOGY DEVELOPMENT

PHYSICAL, CHEMICAL AND MATERIALS SCIENCE
(SCI, ENER, SEC)
- State-of-the-Art Instrumentation and Devices for Precision Electronics, Optics and Microelectronics
- Superconducting and Magnetic Materials
- X-ray Lithography
- Micromachining
- Battery Technology
- Permanent Magnets
- ADesigner≡ Polymers
- Flat Planar Optic Displays

ACCELERATOR TECHNOLOGY
(SCI, SEC)
- High-Field, High-Quality Superconducting Magnets
- High-Power Radio Frequency Systems
- Ultrahigh Vacuum Systems
- Advanced Accelerator Designs
  - High-Gradient Acceleration
  - High-Beam Current Acceleration
  - Novel Structures for Synchrotron Radiation Generation, FELs
  - Novel Particle Beam Diagnostics
- Accelerator/Spallation Source Applications
- Insertion Device Development: Wigglers and Undulators
- High-Power, Short-Pulse Lasers

ENVIRONMENTAL AND CONSERVATION TECHNOLOGIES
(SCI, ENV, ENER, SEC)
- Environmental Remediation and Mitigation
- Energy-Efficiency Technologies
- Waste Treatment
- Disposal of Nuclear Materials
- Radiation Protection
- Infrastructure Modernization
- Transportation: Intelligent Transportation System, MAGLEV
- Ultra Sensitive Detection and Characterization

MEDICAL TECHNOLOGIES
(SCI)
- Biomedical Applications of Nuclear Technology
- Development and Production of Radionuclides/ Radiopharmaceuticals
- Development of Particle Radiation Therapies for Cancer
- Medical Imaging
- X-ray Microbeam Therapy

BIOTECHNOLOGY
(SCI)
- Neutron and Synchrotron X-ray Scattering
- Large-Scale Genome Sequencing
- High-Resolution Scanning and Cryo Electron Microscopy
- Cloning, Expressing and Engineering Genes
- Metal Cluster Compounds for Electron Microscope Labels
- Phage Displays for Probing Specific Interactions

SAFETY, SAFEGUARDS, AND RISK ASSESSMENT
(SEC, SCI, ENV, ENER)
- Safeguards, Nonproliferation and Arms Control
- Safety Analysis of Complex Systems
- Probabilistic Risk Assessment and Management
- Human Reliability
- Material and Component Survivability Testing
- Remote Sensing of Chemical Signatures
- Technical Support for U.S. Policy
- Energy Systems Modeling and Assessment
- Biological and Chemical Weapons Detection and Mitigation

KNOWLEDGE TRANSFER

EDUCATING FUTURE GENERATIONS OF SCIENTISTS AND ENGINEERS
(SCI, ENV, ENER, SEC)

- Scientific Publishing, Lecturing, Conference Participation
- Visiting Scientist Program
- Accelerator Fellowship Program
- Postdoctoral Research Associates
- Engineering Intern Program
- Graduate Student Thesis Projects
- Adjunct Teaching Appointments at Local Colleges
- Office of Educational Program
  - Precollege and College Programs for Students and teachers

EDUCATING THE GENERAL PUBLIC
(SCI, ENV, ENER, SEC)

- Science Museum and Laboratory Tours (20,000 people/year)
- Speakers Bureau
- BNL Videos
- Laboratory Lectures for the Public
- Community Outreach Programs
- School Mentoring Program

TECHNOLOGY TRANSFER
(SCI, ENV, ENER, SEC)

- Scientific Publishing
- Industrial Users at the Research Facilities
- Consulting by Scientific Staff for Industry
- Technology Transfer Office
  - Patenting and Licensing of BNL Inventions
  - Technical Assistance for Industry
  - CRADAs
  - Personnel Exchange Program with Industry
  - Research Partnerships with Industry
  - Industry-Sponsored Proprietary Research and Development

INFORMATION TECHNOLOGY
(SCI, ENV, ENER, SEC)

- Electronic Library and Database Information Source
- Networking - "Information Superhighway"
- Technical and Scientific Publishing
- National Nuclear Data Center
- Protein Data Bank
- Data Visualization
- ALARA Center

TRAINING AND EDUCATION OF TECHNOLOGISTS
(SCI, ENER, SEC, ENV)

- Safety of Soviet-Designed Reactors
- Safeguards of Special Nuclear Materials in the former Soviet Union
- Mentoring within the DOE Complex
- Waste Management in the former Soviet/Arctic Regions

Management Process

PROGRAM DESCRIPTION:

Introduction: The Department of Energy's (DOE) Laboratory Directed Research & Development (LDRD) Program at Brookhaven National Laboratory (BNL) was originally established as the "Exploratory Research Program" under the guidelines set forth in DOE Order 5000.1 in May 1984. From inception through September 2000, a period spanning sixteen fiscal years, the Laboratory has authorized $44.0 million in Exploratory R&D, consisting of 226 separate projects.

BNL LDRD PROGRAM HISTORY 1985-2000

FISCAL YEAR	AUTH K$	COSTED K$	NO. REC'D	NEW STARTS
1985	1,842	1,819	39	13
1986	2,552	2,515	22	15
1987	1,451	1,443	29	8
1988	1,545	1,510	46	14
1989	2,676	2,666	42	21
1990	2,008	1,941	47	9
1991	1,353	1,321	23	14
1992	1,892	1,865	30	14
1993	2,073	2,006	35	14
1994	2,334	2,323	44	15
1995	2,486	2,478	46	13
1996	3,500	3,050	47	17
1997	4,500	3,459	71	10
1998	4,000	2,564	53	4
1999	4,612	4,526	67	25
2000	6,000*	---	93	20
TOTALS	44,046	35,524	734	226

*Additional projects may be funded in FY 2000, pending the availability of funds.

Historical Perspective: Brookhaven National Laboratory was established in 1946. Throughout its history, certain projects of an exploratory nature, sometimes referred to in the past as "seed money projects," were supported with overhead funding. In 1979, as a result of a Review Audit in that year, the seed money accounting procedures were formalized, and oversight by the then DOE Brookhaven Group Manager was first established. This seed money program operated at a variable level of funding, which averaged about 0.1 percent of the Laboratory's operating budget over the period 1979 to 1984.

In May 1984, the program was expanded. The expanded program embraced the new Exploratory R&D guidelines of DOE Order 5000.1. The new program, called the Exploratory Research Program, was put into effect for FY 1985 funding. The current Laboratory Directed Research & Development Program reflects the operating styles and many of the procedures of the earlier programs, which have evolved somewhat informally over the years. It also encompasses the requirements of the current DOE Order 413.2.

Goals and Objectives: The goals and objectives of BNL's LDRD Program can be inferred from the Program's stated purposes. These are to (1) encourage and support the development of new ideas and technology, (2) promote the early exploration and exploitation of creative and innovative concepts, and (3) develop new "fundable" R&D projects and programs. The emphasis is clearly articulated by BNL to be on supporting exploratory research "which could lead to new programs, projects, and directions" for the Laboratory.

General Characteristics of the LDRD Program: Projects or studies that are appropriate candidates for the Laboratory's LDRD Program include, but are not limited to, (1) projects, normally relatively small, in the forefront areas of basic and applied science and technology for the primary purpose of enriching laboratory capabilities, (2) advanced study of new hypotheses, new concepts, or innovative approaches to scientific or technical problems, (3) experiments and analyses directed toward "proof of principle" or early determination of the utility of new scientific ideas, and (4) conception and preliminary technical analysis of experimental facilities or devices.

PROGRAM ADMINISTRATION:

Overall Coordination: Overall responsibility for coordination, oversight, and administration of BNL's LDRD Program resides with the Laboratory's Director. The Office of the Assistant Laboratory Director for Finance & Administration assists in the administration of the program. This includes administering the program budget, establishment of project accounts, maintaining summary reports, and reports of Program activities to the DOE through the Brookhaven Group Manager.

Responsibility for the allocation of resources and the orchestration, review, and selection of proposals lies with a management-level group called the Laboratory Directed Research & Development Program Committee.

The Program Committee is made up of ten members. For Fiscal Year 1999, the Laboratory's Deputy Director for Science & Technology is the chairperson of the Committee. The other members are the four Associate Directors of the Laboratory, as well as four members from the scientific departments and divisions, and the Assistant Director for Finance & Administration.

1999 LDRD PROGRAM COMMITTEE
(for Selection of 2000 Programs)

Peter Paul	**Chairperson**
Robert Bari	**Advanced Technology**
Steve Dewey	**Chemistry**
Teresa Fryberger	**Applied Science & Technology**
Thomas Kirk	**High Energy & Nuclear Physics**
Denis B. McWhan	**Basic Energy Sciences**
Mike Murtagh	**Physics**
Satoshi Ozaki	**RHIC**
Veljko Radeka	**Instrumentation**
Brian Sack	**Finance & Administration**

Allocating Funds: There are two types of decisions to be made each year concerning the allocation of funds for the LDRD Program. These are: (1) the amount of money that should be budgeted overall for the Program; and (2) of this, how much, if any, should go to each competing project or proposal. Both of these decisions are made by high-level management.

Concerning the overall budget, for each upcoming fiscal year the Laboratory Director, in consultation with the Assistant Laboratory Director for Finance & Administration, develops an overall level of funding for the LDRD Program. The budget amount is then incorporated into the Laboratory's LDRD Plan which formally requests authorization from the DOE to expend funds for the LDRD Program up to this ceiling amount.

The majority of projects are authorized for funding at the start of the fiscal year. However, projects can be authorized throughout the fiscal year, as long as funds are

available and the approved ceiling for the LDRD Program is not exceeded.

The actual level, which may be less, is determined during the course of the year and is affected by several considerations including: the specific merits of the various project proposals, as determined by Laboratory management and the members of the LDRD Program Committee; the overall financial health of the Laboratory; and a number of budgetary tradeoffs between LDRD and other overhead expenses. At BNL the LDRD Program has historically amounted to a much smaller portion of the total budget area than at comparable national labs. This prevented the Laboratory from preparing itself for work in emerging areas of research. Accordingly, this fraction of LDRD funds is being increased with a target of about 4%.

LDRD COSTS VS. TOTAL LABORATORY COSTS

operating $ in millions

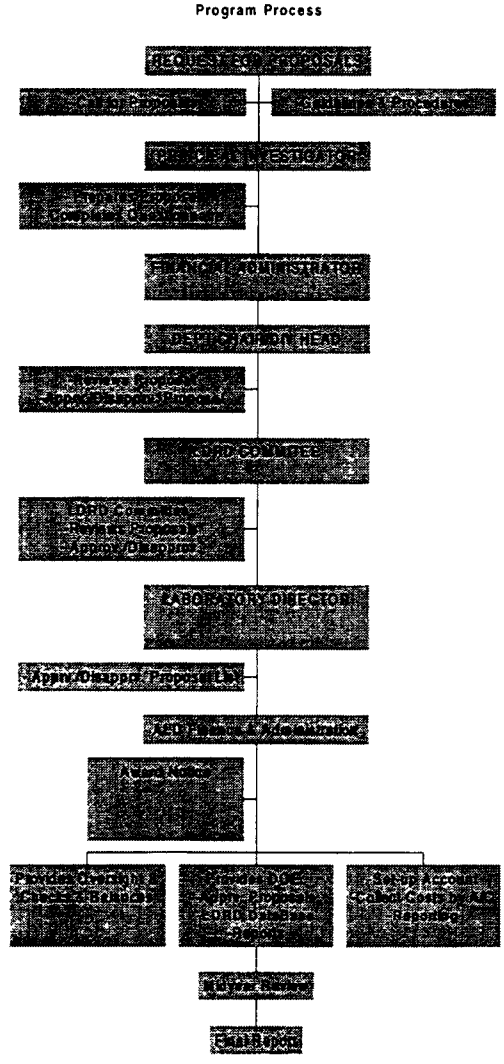
FISCAL YEAR	DOE FUNDS	WFO FUNDS	TOTAL FUNDS	LDRD FUNDS	% OF TOTAL
1985	153.0	40.4	193.1	1.82	0.9
1986	156.5	45.1	201.6	2.52	1.2
1987	161.7	45.6	207.3	1.44	0.7
1988	176.7	45.9	222.6	1.51	0.7
1989	193.6	46.7	240.3	2.67	1.1
1990	203.8	45.2	249.0	1.94	0.8
1991	220.9	50.3	271.2	1.32	0.5
1992	234.3	47.2	281.5	1.87	0.7
1993	231.4	47.3	278.7	2.01	0.7
1994	237.0	47.9	284.9	2.32	0.8
1995	243.0	53.7	296.7	2.48	0.8
1996	251.6	50.6	302.2	3.05	1.0
1997	257.2	52.5	309.7	3.46	1.1
1998	251.8	49.5	301.3	2.56	.8
1999	294.1	48.1	342.2	4.53	1.3
2000	343.0	58.0	401.0	6.00	1.5

Concerning the allocation of resources to specific topic areas or to individual project proposals, such issues are addressed on a case-by-case basis by the LDRD Program Committee, once specific proposals have been received. The Committee meets periodically to review and recommend project proposals and to determine the amount of funding to be made available to the LDRD Program. The requirements of DOE Order 413.2 are carefully considered during the selection process to ensure that proposals are consistent with DOE's criteria.

Request for Proposals: The availability of special funds for research under the LDRD Program is well publicized throughout the Laboratory. This is done using two methods --one occurring at yearly intervals, the other occurring irregularly. Each year a call memo is sent by the Laboratory Director to all scientific staff issuing a "call for proposals." For FY 2001 this call memo will be issued in January. This early schedule will better facilitate the recruitment of post-doctorate students to support LDRD projects. This memo is accompanied by a document entitled, "Guidelines and Procedures for Developing Proposals via the Laboratory Directed Research and Development (LDRD) Program." The other method is by announcement in the Brookhaven Bulletin, the Laboratory's weekly newspaper.

The "Guidelines and Procedures" document specifies the requirements necessary for participation in the program. It states the program's purpose, general characteristics, procedures for applying, and restrictions. An application for funding, i.e., a project proposal, takes the form of a completed "Proposal Information Questionnaire." An application must be approved up the chain-of-command which includes the initiator's Department or Division Budget Administrator, and the Department Chairperson or

Division Head. Plans to ensure the satisfactory continuation of the principal investigator's regularly funded programs must also be approved. The applications are then forwarded to the LDRD Program Committee for full review and consideration for funding.



The process that solicits and encourages the development of proposals has evolved into two modes of operation. Specifically, the ideas for proposal development may originate among the scientific staff in response to the general call for proposals. Alternatively, they may be initiated by Laboratory science management. Eventually, both follow the standard procedures for proposal approval up the chain-of-command to the same decision makers. The fact that all proposals must be approved up the chain-of-command permits BNL managers to consider all ideas together when designing the mix of projects for the LDRD Program.

An initiative from management typically takes the form of a broad topical area or item of special interest. Then ideas are communicated to a group of scientific staff, who are known to be in a position to pursue and develop the idea in the form of a more formal proposal.

Proposal Review: Once a proposal is approved by the cognizant line managers, all proposals are forwarded to the Chairperson of the Committee who transmits a copy of all proposals received to the Committee for review. The Committee considers all proposals that have met certain minimum requirements pertaining to the Department's and BNL's LDRD policies.

Lead responsibility of a proposal is assigned to that member of the Committee who oversees and directs the technical area from which the proposal originated. All members have several weeks to review the proposals and prepare for the full debate of the proposal.

Formal peer reviews, consisting of written comments by experts outside the normal lines of supervision, are not usually performed. The members of the Committee are considered to have sufficient technical knowledge so that peer reviews are seldom required. If additional information is needed, the Principal Investigator of a proposal makes a presentation to the full Committee.

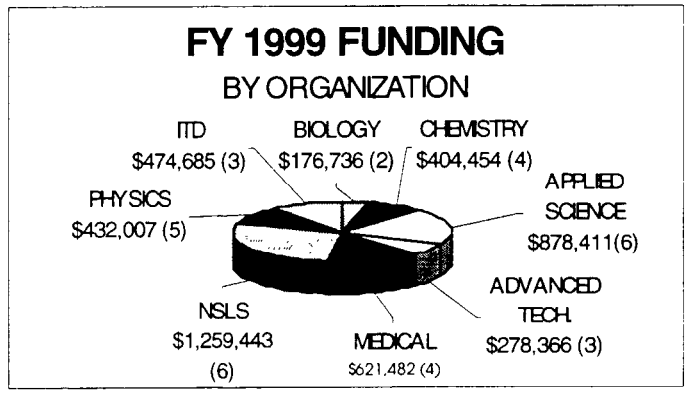
Selection Criteria: Minimum requirements of each proposal are: (1) consistency with program purpose; (2) consistency with missions of BNL, DOE, and NRC; (3)

approval by Department Chair-person and/or Division Head, and cognizant Associate/ Assistant Director; (4) assurance of satisfactory continuation of principal investigator's regularly funded programs; (5) modest size and limited to 3 years; (6) will not substitute for, supplement, or extend funding for tasks normally funded by DOE, NRC, or other users of the Laboratory; (7) will not require the acquisition of permanent staff; (8) will not create a commitment of future multi-year funding to reach a useful stage of completion; and (9) will not fund construction line-item projects, facility maintenance, or general purpose capital equipment.

The selection criteria used to evaluate and rank individual proposals are stated in broad terms. While the "Guidelines and Procedures" document clearly states that selection is based on (1) scientific or technological merit, (2) innovativeness, (3) compliance with minimum requirements, (4) proposal cost as compared to the amount of available funding, and (5) its potential for follow-on funding. The requirements of DOE Order 413.2 are also carefully considered during the selection process to ensure that proposals are consistent with DOE criteria.

Project Approval: After all presentations are heard, the Committee selects the highest priority proposals by concurrence. Differences, if any, are resolved by the Chairperson. Some funding may be held in reserve during the earlier meetings of the fiscal year so that funds remain available for proposals submitted at later dates. The funding amount requested in any one specific proposal may be changed or adjusted during the approval process. The Committee's recommendation is then submitted to the Director for his approval.

The Assistant Laboratory Director for Finance & Administration then sets up a separate Laboratory overhead account to budget and collect the costs for the project. Statistics on the number of projects approved, compared to those rejected, show an overall approval rate of about 31 percent for new starts. Eight scientific departments were represented in the FY 1999 LDRD Program. From inception of the program through September 1999 (for FY 2000), 734 project proposals were considered and 226 were approved.



Project Supervision: Supervision over the actual performance of LDRD projects is carried out in the same way as other research projects at the Laboratory. Each principal investigator is assigned to an organizational unit (Department, Division), which is supervised by a chairperson or manager.

Each chairperson or manager is responsible for seeing that the obligations of the principal investigator are satisfactorily fulfilled and that the research itself is carried out according to standard expectations of professionalism and scientific method. The chairperson or manager is kept informed of the project's status, schedule, and progress.

A mid-year review of all projects is performed by the chairperson of the LDRD Program Committee. This review checks on the progress of the projects including its funding schedule.

The chairperson or manager ensures that the work is completed in a timely manner and that annual status reports are submitted to the Director.

In addition, LDRD Program activity is reported to the DOE Brookhaven Group Manager, including copies of all funded proposals, a LDRD Program data base, and a project funding and schedule summary report.

Project Reporting: Routine documentation of each project funded under the LDRD Program consists of a file containing: (1) a copy of the written proposal; (2) all interim status reports; (3) notifications of changes in research direction, if any; and (4) reports on cost incurred. Also, a formal Annual Report on the LDRD Program is submitted to BNL management and the DOE, summarizing work progress, accomplishments, and project status on all projects.

Documentation for the overall Program consists of (1) various program history files, (2) a running list of all proposals with their acceptance/rejection status, (3) funding schedule and summary reports for all approved projects, (4) permanent records on cost accounting, and a data base containing information on each funded project (description, funding by fiscal year, status and accomplishments, follow-on funding, publications, etc.).

Some of the projects involve animals or humans. Those projects have received approval from the Laboratory's appropriate review committees. The projects which involve animals or humans are identified in this report as follows:

Note: This project involves animal vertebrates or human subjects.

This is noted on the summary sheet and also at the end of each report.

ALIGNMENT WITH DOE'S MISSION:

BNL is committed to mount programs (including the LDRD) of the highest quality that address DOE's Strategic Missions. Of the Four Businesses identified in the Secretary of Energy's Strategic Plan, Brookhaven National Laboratory contributes most strongly to Science and Technology.

While maintaining traditional strengths in science and technology, BNL intends to participate more effectively in the other three business areas defined by DOE: Energy Resources, National Security, and Environmental Quality.

Brookhaven National Laboratory's FY 1999 LDRD Program covered the following DOE mission areas.

Programs/Projects	Funding $000
Science & Technology	$3,911
Environmental Quality	540
Energy Security	0
National Security	75
TOTAL	$4,526

SUCCESS INDICATORS:

Overall the BNL LDRD Program has been very successful. Some of the more common indicators/measures of success are: 1) amount of follow-on funding, 2) the number of patents applied for, and 3) the number of full-length pages published in other journals or publications.

An analysis of FY 99 projects shows that 1) Seven of the projects reported that proposals/grants resulted in funded programs funded or submitted for funding, 2) Twenty-three articles or reports were reported to be in publication or submitted for publication.

Summary of FY 1999 LDRD Program

In FY 1999, the BNL LDRD Program funded 33 projects, 25 of which were new starts, at a total cost of $4,525,584. Following is a table which lists all of the FY 1999 funded projects and gives a history of funding for each by year.

Several of these projects have already experienced varying degrees of success as indicated in the individual Project Program Summaries which follow. A total of 29 informal publications (abstracts, presentations, reports and workshop papers) were reported and an additional 23 formal (full length) papers were either published, are in press or being prepared for publication. The investigators on five projects have filed for patents.

Seven of the projects reported that proposals/grants had either been funded or were submitted for funding. The complete summary of follow-on activities is as follows:

Follow-on Activity of LDRD Projects	
	Number of Projects
Informal Publications	**29**
Formal Papers	**23**
Grants/Proposals/Follow-on Funding	**7**

In conclusion, a significant measure of success is already attributable to the FY 1999 LDRD Program in the short period of time involved. The Laboratory has experienced a significant scientific gain by these achievements.

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT
FY 1999 APPROVED PROJECTS

				Actual Cost			Budget	Requested		Account
Proj No	PROJECT TITLE	P. I.	Dept	FY 97	FY 98	FY 99	FY 00	FY 01	Total	Number
97-02	Physics Goals for a New Intense Muon Facility	W. Marciano	PHYS	91,434	99,545	12,045			394,003	2690
97-44	X-ray Schlieren Computed Tomography	A. Dilmanian	MED	59,792	94,212	42,789			350,797	2663
97-50	Development of Pump-and-Probe Lidar for the In Situ Study of Fast Atmospheric Chemical Reactions	A.J. Sedlacek, III	DAT	99,066	99,778	93,980			491,668	2682
97-68	Center for Imaging in Drug Abuse Research	N.D. Volkow	MED		332,828	341,508			1,007,164	2664
98-23A	Performance Enhancement In a Photoinjector Electron Linac	E.Johnson	NSLS			300,339	266,000	300,000	866,339	2624
98-23B	Pulse Compression and Emittance Preservation in a High Brightness Electron Linac	W. Graves	NSLS			150,621	134,000	150,000	434,621	2624
98-27	Novel Mechanisms of Hydroxy Fatty Acid Biosynthesis	J. Shanklin	BIO		99,646	101,881			301,173	2684
98-58	Sensitive Detection and Rapid Identification of Biological Agents by Single Molecule Detection	M. Wu	DAT		100,787	99,618			301,192	2683
99-01	Ultra-fast Dectector based on Optical Techniques	Y. Semertzidis	PHYS			113,345	90,000	125,244	418,589	2688
99-03	NOVA: Networked Object-Based enVironment for Analysis	T. Wenaus	PHYS			99,894	80,000		259,894	2689
99-05	Aerosol Module for Climate Models Using Advanced Computer Techniques	C. Benkovitz	DAS			98,887	80,000		258,887	2604
99-06	Environmental Carbon Observatory (ECO)	G. Hendrey	DAS			346,926	240,000	727,000	1,553,926	2607
99-10A	Parallel Algorithms for Accelerator Design	J. Glimm	DAS			125,805	170,000	370,000	665,805	2605
99-10B	Photonic Band Gaps in Nanostructured Materials	J. Davenport	DAS			95,000	140,000	296,000	531,000	2605
99-10C	Parallel Algorithms for Biomedical Image Processing	J. Davenport	DAS			125,000	180,000	392,000	697,000	2605
99-26	Electron Diffraction Studies of Charge Ordering in Transition-Metal Oxides	Y. Zhu	DAS			86,793	70,000	120,000	346,793	2606
99-28	Evaluation of a Millimeter Quasi-Optical Source for Non-Destructive Detection & Analysis	M. Ruckman	DAT			84,768	60,000	120,000	324,768	2603
99-40	Microdistribution Studies of Boron 10 B for Boron Neutron Capture Therapy Using Transmission Electron Microscopy	R. Ma	MED			117,614	60,000		237,614	2610
99-41	Efficasy of Unidirectional Microbeam Radiation Therapy in Treating Malignant Tumors: Preclinical Studies in Rats and Mice	A. Dilmanian	MED			119,571	130,000		379,571	2611
99-45	Toxin Bio-information Resource	S. Swaminathan	BIO			74,855	75,000		224,855	2633
99-46	Experimental and Theoretical Investigation of Transition Metal Oxides	J. Hill	PHYS			84,381	60,000		204,381	2687
99-48	Pulsed Laser Deposition Facility	P. Johnson	PHYS			122,342	60,000		242,342	2686
99-50	Ultrashort Electron Bunch Length Monitor	W. Graves	NSLS			110,200	65,000		240,200	2619
99-51A	High Gain FEL Amplifier	G. Rakowsky	NSLS			100,000	100,000	409,000	609,000	2620
99-51B	Deep Ultra-Violet Free Electron Laser Optimization	E. Johnson	NSLS			396,890	300,000	136,000	832,890	2620
99-53	Development of High Brightness Electron Sources	I. Ben-Zvi	NSLS			201,393	200,000	250,000	851,393	2623
99-56	Attosecond Pulse Generation in High Harmonics	L. DiMauro	CHEM			109,251	80,000	75,000	344,251	2658
99-57	Development of a 2-D Ion Imaging Detector for VUV-FEL Applications	M. White	CHEM			98,803	80,000		258,803	2657
99-59	Application of Quantitative MRI: Water Concentration and Blood-Brain-Barrier Permeability in Multiple Sclerosis	W. Rooney	CHEM			74,443	75,000	75,000	299,443	2669
99-62	In Situ Time Resolved Studies of Catalysts for SOx and NOx Decomposition using Synchrotron Radiation	J. Rodriguez	CHEM			121,957	50,000	120,100	342,057	2656

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT
FY 1999 APPROVED PROJECTS

				Actual Cost			Budget	Requested		Account
Proj No	PROJECT TITLE	P. I.	Dept	FY 97	FY 98	FY 99	FY 00	FY 01	Total	Number
99-63A	Advance Object Oriented Databases on Linux Systems	D. Stanpf	ITD			114,685			114,685	2608
99-63B	Mobile Agent Based Monitoring of Distributed Computing Systems	R. Ibbotson	ITD			180,000			180,000	2608
99-63C	Demonstration of Advanced Commercial Ethernet Technology	T. Healy	ITD			180,000			180,000	2608
		TOTAL				4,525,584	2,845,000	3,665,344		

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

1999 PROJECT PROGRAM SUMMARIES

Physics Goals For a New Intense Muon Facility

William J. Marciano *97-02*

PROJECT DESCRIPTION:

The focus of this project is to identify and scrutinize the most compelling physics studies that could be carried out at a new very intense muon source capable of delivering $10^{11} \sim 10^{13}\mu^{\pm}$/sec, 4 to 6 orders of magnitude beyond current facilities available at TRIUMF and PSI. Such a source could be developed in the near term at Brookhaven's AGS, be part of the front end of a future muon collider complex, or be coupled to an intense neutron spallation source.

To motivate the new intense muon source, we have outlined a program of experiments that could be carried out there. The program would initially concentrate on fundamental elementary particle physics studies, but later find applications in condensed matter via μSR, biology where μ^+e^- atoms could be used as probes and muon catalyzed fusion research. Some of the fundamental measurements envisioned include:

1. Precision Measurements of Muon Properties (τ_μ, g-2, e.d.m., muonium *hfs* etc.)
2. Muon Neutrino Studies (mass, oscillations...)
3. Searches for *P*- and *T*- violation in Muonic Atoms
4. Searches for Muon-Number Non-Conservation

Each of these topics has undergone close scrutiny to assess its potential importance and likelihood for uncovering "New Physics."

TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

To date, much of the LDRD effort has been directed at studies of the muon-number violating reaction μ^- + Nucleus $\rightarrow e^-$+ Nucleus. The basic concept is simple, a stopped μ^- will quickly cascade into a $1s$ atomic orbit and reside in close contact with the nucleus. There it lives of order 10^{-6} sec. before either undergoing capture $\mu^- p \rightarrow \nu_\mu n$ or decay $\mu^- \rightarrow e^- \nu_\mu \bar{\nu}_e$. If, however, muon-number is not exactly conserved, the coherent reaction $\mu^- N \rightarrow e^- N$ becomes possible. Its signature, a monoenergetic e^- with $E_e \cong 105$ MeV is very distinct from backgrounds and relatively easy to identify. Already, experiments have searched for that rare reaction and set an upper bound of 7×10^{-13} on its occurrence. With an AGS source capable of delivering $10^{11}\mu^-$/sec, one could probe the 10^{-16} level. Recognizing that fact, a proposal (P940, W. Molzon *et al.*) was submitted to BNL with the goal of searching for $\mu^- Al \rightarrow e^- Al$ to better than 5×10^{-17} and received scientific approval. That proposal has now been submitted to the NSF as a new special AGS program called RSVP. Because such an experiment detects only one final state particle, it can take very high intensities without encountering accidentals. Hence, we believe it could ultimately be pushed to the $10^{-18} \sim 10^{-19}$ level.

Preliminary feasibility studies of coherent muon-electron conversion were initiated at the 1996 AGS 2000 workshop and at a small but dedicated workshop held in July 1996 at the Institute for Theoretical Physics in Santa Barbara. Following those meetings, collaborative theoretical work with A. Czarnecki and K. Melnikov (Postdocs at Univ. of Karlsruhe) began. During FY97, the transition rate for muon-electron conversion in atoms was carefully examined and detailed computer calculations were carried out for arbitrary muon-number

violating interactions. Relativistic atomic effects, Coulomb wavefunction distortions, finite nuclear distributions, etc. were taken into account for a broad range of stopping targets. The results were published in "Coherent Muon-Electron Conversion in Muonic Atoms" A. Czarnecki, W. Marciano, and K. Melnikov, AIP Conference Proc. 435, Eds. S. Geer and R. Raja (1998).

A second part of the LDRD effort has been studies of new sources of *P* and *T* violation that might be unveiled using muons. Predictions for the muon electric dipole moment (which violates *P* & *T*) were examined in a variety of models. Those studies were done with O. Vives, a postdoc from Spain who visited BNL for 6 months, supported in part by LDRD funding.

In the area of precision muon measurements, several theoretical ideas were developed during FY99. The use of high precision measurements of the muon lifetime combined with the $W^{\pm}$ mass measurement was shown to provide a severe constraint on heavy gauge bosons (W. Maricano, Phys. Rev. **D60**, 093006 (1999)). Bound state and material effects on the muon lifetime were examined (A. Czarnecki, G.P. Lepage and W. Marciano HEP-PH/9908439). Higher order contributions to g_{μ}-2 were refined (A. Czarnecki and M. Skrzypek, submitted to Phys. Lett. B) and a review of leptonic anomalous magnetic moments was prepared (A. Czarnecki and W. Marciano, BNL-HET-98/43 Report).

A related project carried out under some LDRD support involves muon collider Physics studies. W. Marciano in collaboration with B. Kamal (HET postdoc) and Z. Parsa (BNL CAP) examined Higgs resonance signatures and backgrounds at a $\mu^+\mu^-$ collider. Effects due to muon polarization and forward-backward asymmetries were scrutinized. These results have been reported in "Workshop on Physics at the First Muon Collider and at the Front End of the Muon Collider," AIP Conference Proceedings 435 (1998) Eds. S. Geer and R. Raja, p. 657 and "Physics Potential and Development of $\mu^+\mu^-$ Colliders," AIP Conf. Proc. 441 (1998) Ed. D. Cline, p. 174 and p. 347.

ACCOMPLISHMENTS:

The work reported above has led to several concrete developments. Elucidating the importance of μ-*e* conversion for uncovering "New Physics" and scrutinizing its theoretical underpinnings has helped lead to an approved experiment at the AGS (E940, W. Molzon Spokesman) with 5×10^{-17} sensitivity. Studies of the muon e.d.m. provided goals for a future effort at the AGS muon storage ring to push for 10^{-24} *e*-cm sensitivity. A letter of intent for such a measurement has been submitted by Y. Semertzides *et al.*

The renewed interest in low energy muon physics, spawned by this LDRD, has also helped stimulate activities outside of BNL. The RIKEN-RAL muon collaboration has examined upgrading their laboratory to much higher intensities ~ $10^{11}\mu$/sec in an effort to probe fundamental elementary particle measurements. The PSI laboratory in Switzerland has examined the possibility of searching for $\mu^+ \rightarrow e^+\gamma$ at 10^{-14} sensitivity. They have also approved new muon lifetime measurements which have theoretical underpinnings from this LDRD sponsored research.

LDRD FUNDING:

FY 1997	$ 91,434
FY 1998	$ 99,545
FY 1999	$ 12,045

X-ray Schlieren Computed Tomography

F. A. Dilmanian *97-44*
L.D. Chapman
B.A. Dowd
D.P. Siddons
W.C. Thomlinson
In Collaboration with Z. Zhong, B. Ren, X.Y. Wu, T. Bacarian, and I. Orion

PROJECT DESCRIPTION:

A new method of mammography was invented at the National Synchrotron Light Source (NSLS) in 1995 by Chapman, Thomlinson, and their collaborators. The method, initially called X-Ray Schlieren Imaging, is now referred to as Diffraction Enhanced Imaging (DEI). It uses synchrotron-generated, monochromatic, fan-shaped-beam of x-rays for line-by-line imaging of the subject. At the heart of the method is an analyzer crystal, of the same type used in the system's monochromator, which is positioned between the subject and the detector. This geometry rejects x-rays that, when traversing the subject, deviate out of the plane of the fan beam by more than the angular acceptance of the analyzer crystal, and modulates the intensity of those deviating by a smaller angle. The angular acceptance curve, the "rocking curve," typically has 1 width of 1 to 15 microradian. The information on the angular deviation of the transmitted x-rays is used to generate two new images of the subject: a) that of the x-ray index of refraction, and b) that of absorption in which the so-called "x-ray small-angle scattering" is suppressed.

APPROACH:

The goals of the present LDRD have been a) to implement DEI in the computed tomography (CT) mode at the NSLS, b) to use the resulting cross-sectional images to characterize animal tissues, and c) to evaluate the potential of the DEI method in clinical radiography and CT.

PROGRESS:

a. System hardware development

A DEI CT system was established at the X15A beamline of the NSLS. It included the monochromator system of the planar DEI system, and the detector and the data acquisition of the Multiple Energy Computed Tomography (MECT) system. A new tangent arm was developed for improved positioning stability of the analyzer crystal.

b. Routine development

Three sets of CT projection data were acquired, with the analyzer tuned at the rocking-curve's peak, left side, and right side. The data then were analyzed to produce five sinograms, "top," "left," "right," "refraction index," and "apparent absorption," each of which was reconstructed as a CT image. The slice was also imaged with the "conventional" method, i.e. with the analyzer crystal removed.

c. Refractive index images of a phantom

A 50-mm-diameter cylindrical acrylic phantom that included four non-axial cylindrical channels filled with olive oil was imaged at 22 keV. The tilt angles of the channels were 5°, 10°, and 15°. Fig. 1 shows the left, right, and top images, as well as the processed images of "index and refraction" and "apparent absorption." The refraction image is non-zero only at the points in the slice where the beam reached an angulated interface between two different media. We conclude that: a) DEI CT projections can be reconstructed conventionally; b) the refractive-index image is a natural edge-enhancer; c) the image contrast is proportional to the gradient of the refractive index; d) there is a remarkable agreement between the linearity trends of the experimental findings and the theoretical index-of-refraction results.

d. Refractive index images of trabecular bone

The above method was used to image also a piece of bovine trabecular bone at 30 keV. The resulting index-of-refraction image (Fig. 2) had a larger contrast than the conventional CT image, an effect stemming from sharp gradients of the index of refraction at the bone-air interfaces. The method may find application in clinical bone studies to evaluate the "bone quality," a factor that relates to the health risks of osteoporosis.

e. Image of the lungs in mice and rat

A rat and a mouse were imaged at 30 keV and 22 keV, respectively, about an hour after euthanasia. Fig. 3 shows the rat images. The remarkable effect is the high image contrast of the lungs in the "top" images, which stems from the lungs' large amount of small-angle scattering. As a result, the lungs-to-soft-tissue image contrast is reversed. The effect points to the DEI's potential in clinical lung imaging, including detection of pulmonary edema, asthma, and collapsed regions of the lung.

f. Directional effects in muscle images

A 3"-outer-diameter acrylic cup, filled with two pieces of bovine muscle surrounded by water, was imaged at 22 keV (Fig. 4). The muscle fibers were oriented vertically in one piece and horizontally in the other. The "top" image shows a measurable difference between the image contrasts of the two muscle orientations (Fig. 4). The findings signify the first time that directional effects are being observed in radiography. They also suggest that the small-angle scattering in muscle is sizable, and that the amplitude of the small-angle scattering is larger in the direction perpendicular to the lines of muscle fibers.

ACCOMPLISHMENTS:

The program successfully implemented the DEI method in the CT mode, and reached conclusions regarding the potential of DEI in clinical radiography. Although the beam energies used are below those needed for whole-body clinical use, because the image signals both from the refractive index gradients and from the small-angle scattering decline only as the inverse function of the x-ray energy, we expect good DEI image qualities at energies relevant to whole-body clinical radiography and CT (i.e., 40-90 keV). DEI may also find industrial applications in non-destructive testing. A grant proposal on DEI is being prepared for submission to the Office of Biological and Environmental Research (OBER), U.S. Department of Energy.

PAPERS/JOURNALS/PUBLICATIONS:

Dilmanian, F.A. A CT reconstruction algorithms for Diffraction-Enhanced Imaging. Proceeding of the Workshop on Computed Microtomography, 1997 NSLS General Users' Meeting. B. Dowd, Ed.

Dilmanian, F.A.; Zhong, Z.; Ren, B.; Wu, X.Y.; Chapman, L.D.; Orion, I.; and Thomlinson, W.C. Computed tomography using the diffraction-enhanced x-ray imaging method. Poster at the 6th International Conference on Biophysics and Synchrotron Radiation, Argonne, IL, Aug. 4-8, 1998 (Conference Abstract Book, p. 28).

Dilmanian, F.A.; Zhong, Z.; Ren, B.; Wu, X.Y.; Chapman, L.D.; Orion, I.; and Thomlinson, W.C. Computed tomography of x-ray index of refraction using the diffraction-enhanced imaging method. Phys. Med. Biol. 45:933-946, 2000.

Ren, B; Dilmanian, F. A.; Zhong, Z.; Wu, X.Y.; Chapman, D.; and Thomlinson, W.C. Characteristics of lung images from diffraction enhanced x-ray computed tomography. Oral presentation given at the 1999 IEEE Medical Imaging Conference, October 26-29, Seattle, WA.

LDRD FUNDING:

FY 1997	$59,792
FY 1998	$94,212
FY 1999	$42,789

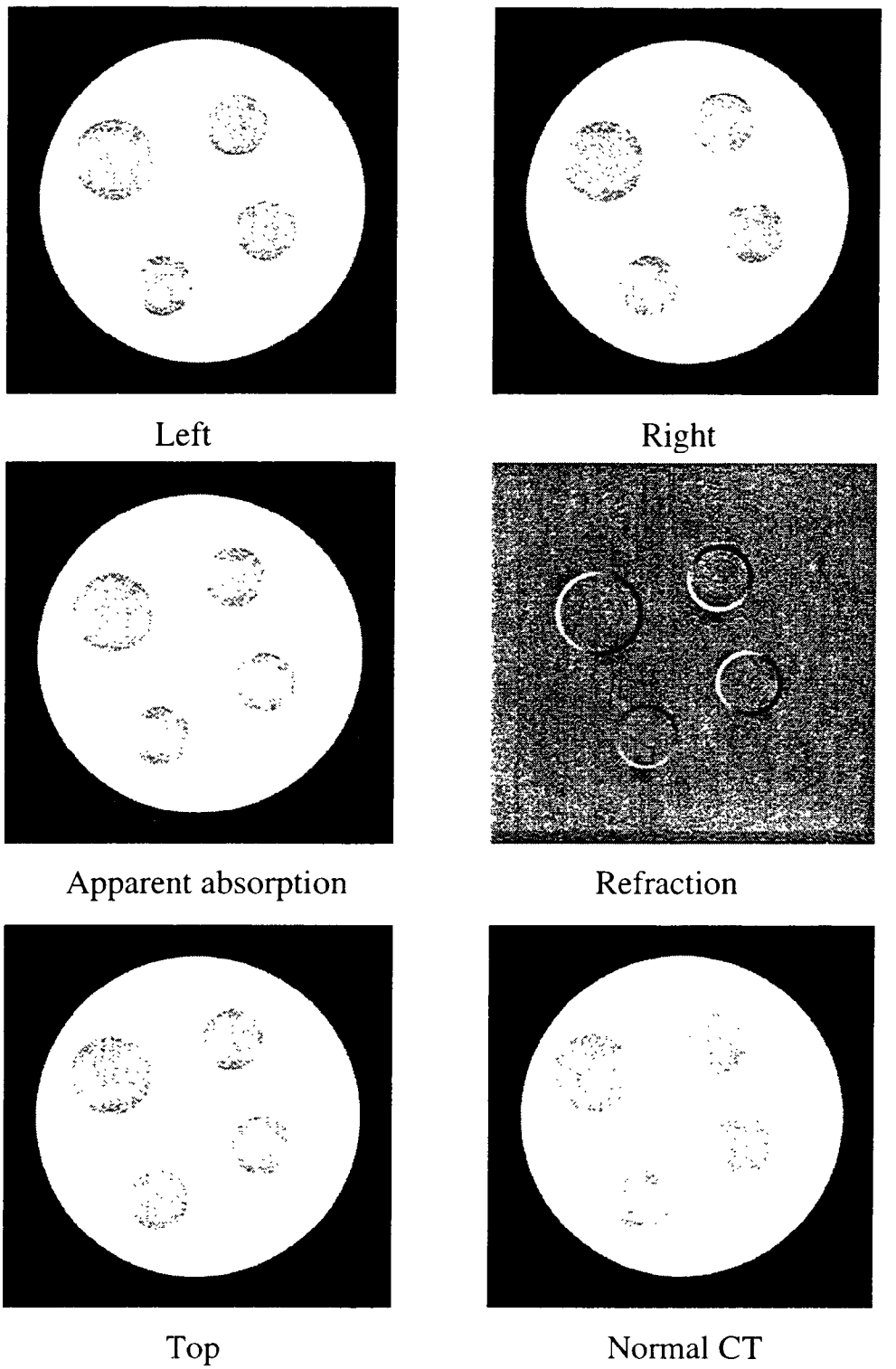


Fig. 1. An acrylic phantom, with oil-filled slanted channels, showing the edge-enhancing effect of the "refraction" image of DEI..

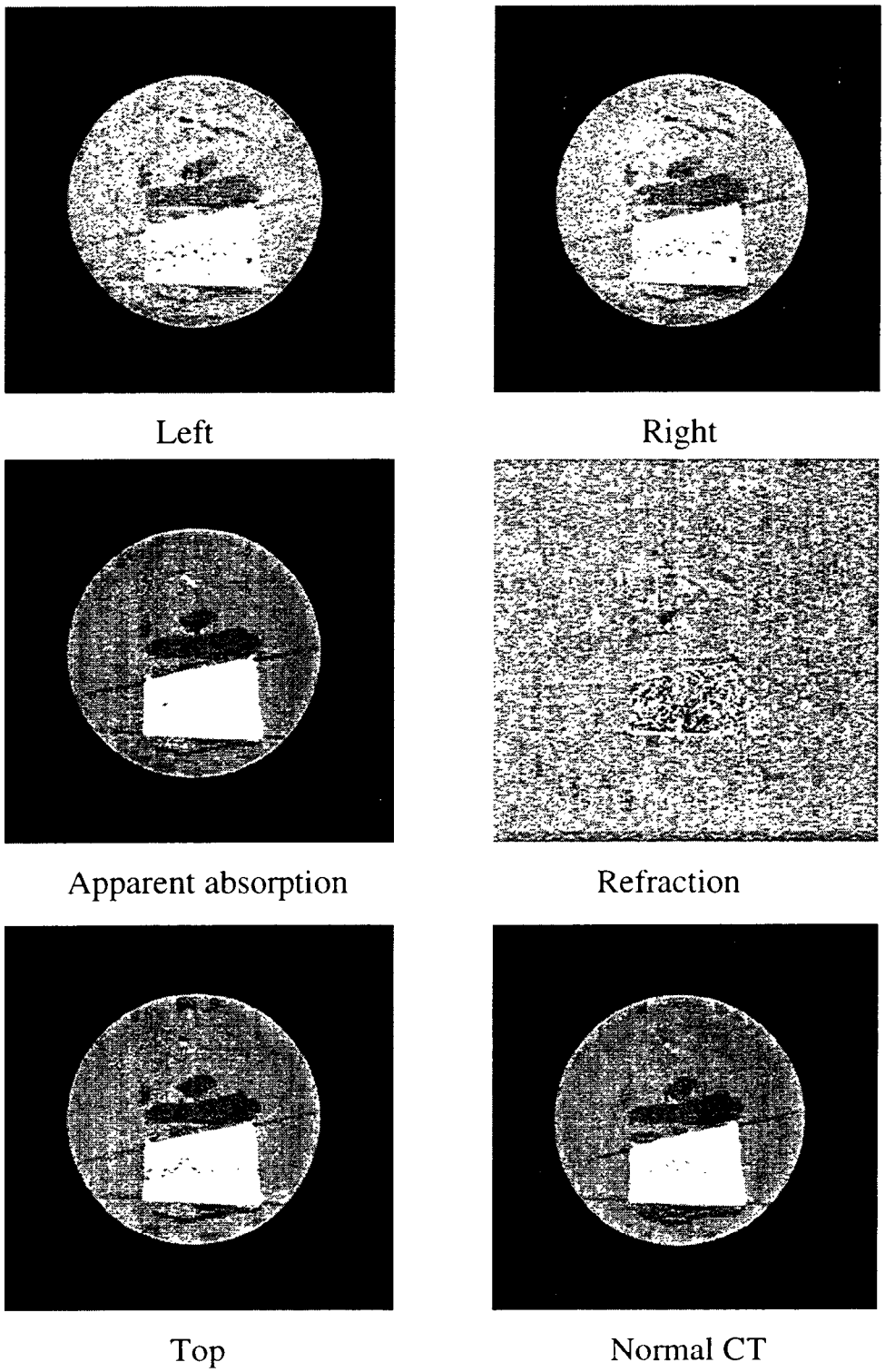


Fig. 2. A cow trabecular bone in a water-filled acrylic tube, showing the edge-enhancing effect of the "refraction" image of DEI.

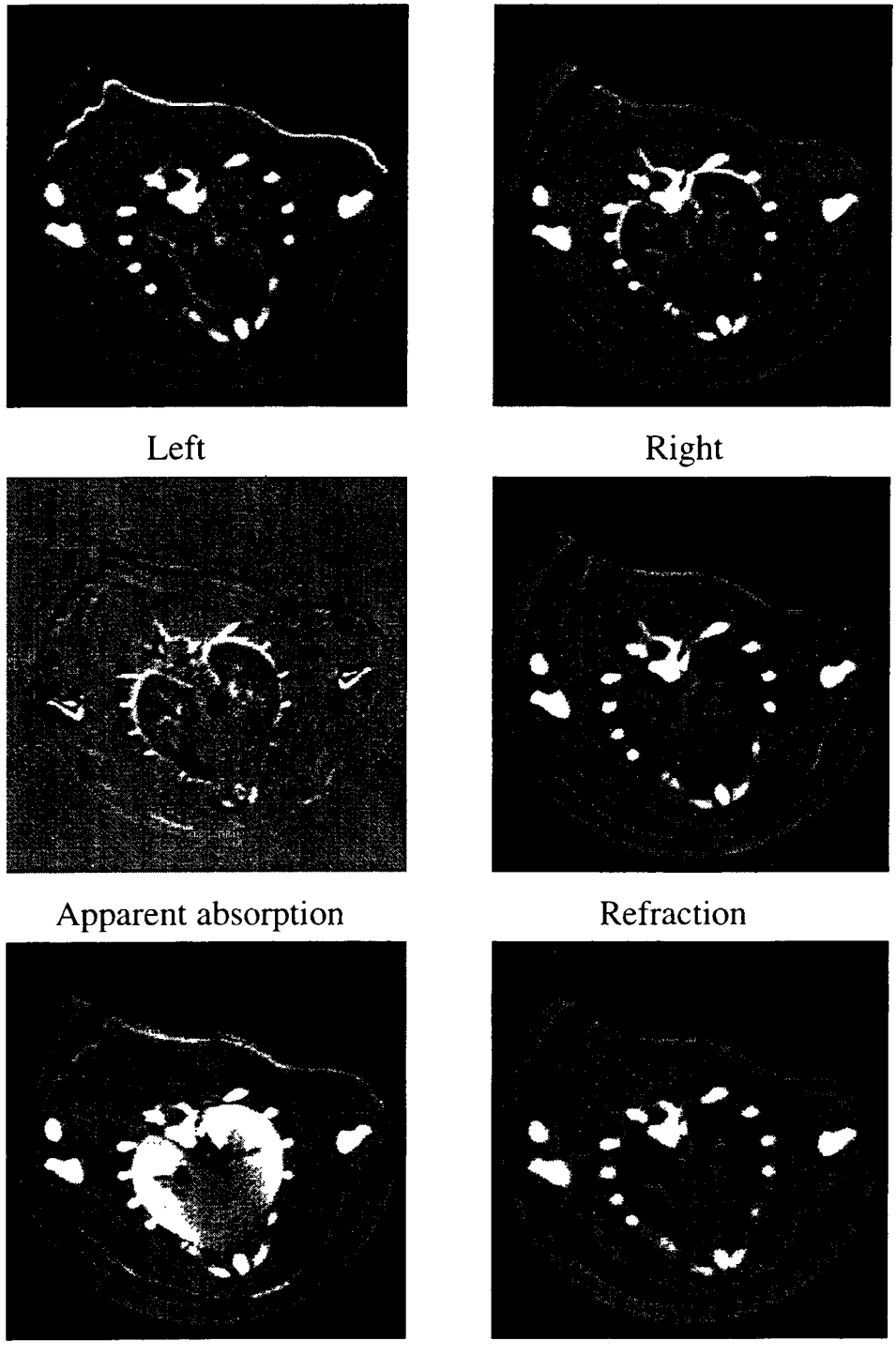


Fig. 3. Rat chest, showing the large image contrast of the lungs in the "top" image of DEI.

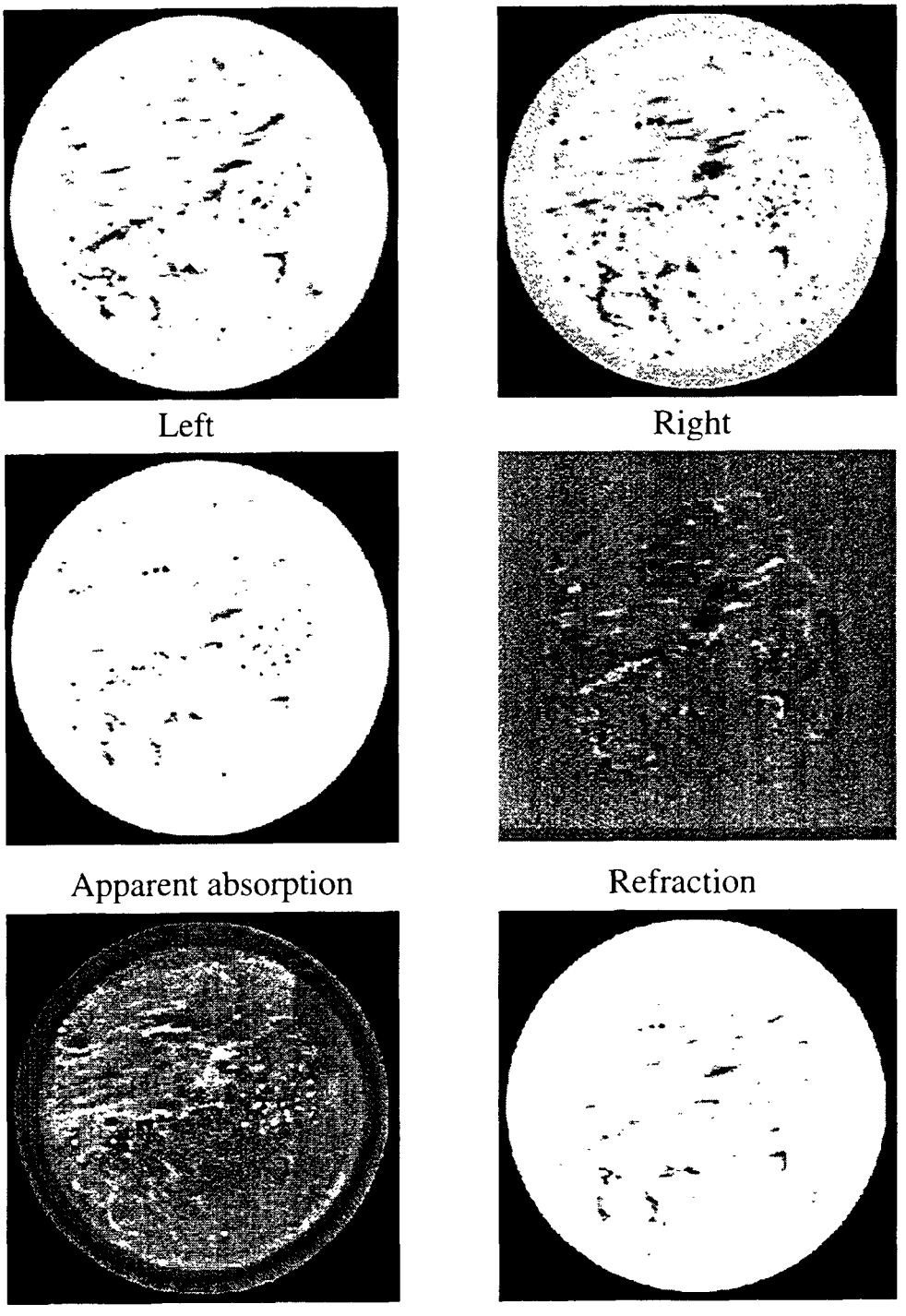


Fig. 4. Two pieces of cow muscle imaged in the perpendicular and parallel directions to the muscle fibers, respectively, showing a difference in the muscle contrasts in the "top" image of DEI.

Development of Pump-and-Probe Lidar for the *In-situ* Study of Fast Atmospheric Chemical Reactions

A. J. Sedlacek *97-50*

PROJECT DESCRIPTION:

Focus for this final year of support was on augmenting DOE/NN supported work on the Mini-Raman Lidar System (MRLS) by addressing fundamental science issues associated with the MRLS. Specifically, since the DOE/NN office was strictly funding instrumentation fabrication and not adequately addressing fundamental scientific issues associated with this novel instrument, it was felt that the tools and expertise developed during the course of this LDRD should be brought to bear on those scientific issues. The scope of work addressed issues including: throughput issues associated with this novel stand-off sensor; detection sensitivity; spectral selectivity; and automated spectral pattern matching.

Background: The Mini-Raman Lidar System (MRLS) is a "proof-of-principle" chemical sensor that combines the spectral fingerprinting of UV Raman spectroscopy with the principles of solar-blind Lidar to open a new venue for the short-range (meters to tens of meters), non-contact detection and identification of unknown substances on surfaces. Emergency response, environmental monitoring/ remediation, materials processing, and forensic investigations often require rapid, *in situ*, real-time detection and identification of small amounts of substances on surfaces. Optical spectroscopic methods are well-suited for this task, as evidenced by the availability of portable chemical sensors based on laser-induced fluorescence, infrared absorption, and Raman scattering.

The Mini-Raman Lidar System represents a distinctly different venue in Lidar. Although the MRLS borrows the basic design of Lidar systems, it breaks from the conventional paradigm of Lidar in that it is designed specifically for detection of substances on surfaces at ranges of fifty meters or less. Typically, Lidar is used to detect air-borne substances at ranges on the order of kilometers. When fully developed, the MRLS has the potential of moving Lidar technology from the domain of a small number of highly-trained specialists into the hands of a large number of first responders, such as police, firemen, and hazardous materials technicians.

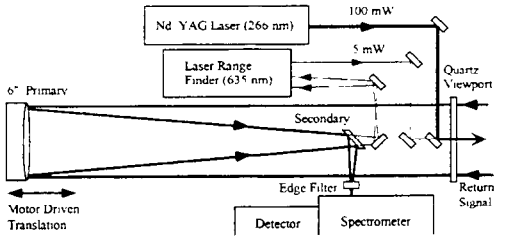
PREVIOUS TECHNICAL PROGRESS – Fiscal Year 1998:

LDRD activities during FY97 and FY98 focused on the development of the RaDIAL technique which uses the inelastic Raman scattering returns from atmospheric nitrogen and oxygen as the two *in situ* probing wavelengths for the DIAL-like measurement. In the RaDIAL technique one of the Raman returns is tuned to the peak of the molecular absorption and the other to a non-absorbing region. By taking advantage of the constancy of the number density ratio of atmospheric nitrogen molecules to atmospheric oxygen molecules and knowing the nitrogen and oxygen Raman cross sections, the concentration of scattering species can be determined. Hence, the N_2 and O_2 Raman returns provide an *in situ* calibration standard. The N_2 and O_2 Raman beams for the differential measurement take place at the same time, in the same spatial volume, and the beams are transmitted through the same atmospheric (turbulence)

structure. The RaDIAL technique addresses traditional concerns of the DIAL technique such as atmospheric turbulence, aerosol burden and laser shot-to-shot energy variations since classical DIAL monitors only the elastically scattered return signals. RaDIAL offers a superior stand-off sensing technique where range-resolved, open-path applications are required.

TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

Approach: Research carried in FY99 utilized a 2nd-generation mini-Raman Lidar system. Shown in Figure 1, this chemical sensor consists of a 50 lb. tripod-mounted optical head, which is connected, via an umbilical cord, to a power supply cart. Figure 1 also shows a schematic of the optical head, which contains both the transmitter and receiver housed within a weatherproof case. The entire optical system is mounted rigidly to a single platform to preserve the alignment of all of the components.



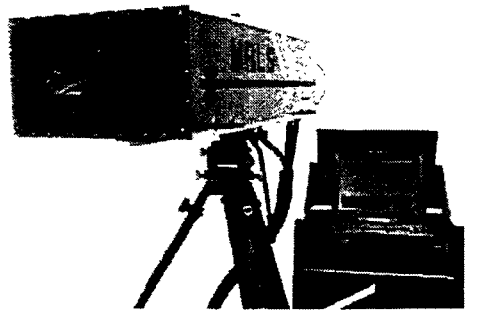


Figure 1. Schematic of the Mini-Raman Lidar System (MRLS) and photo of MRLS.

Technical Progress and Results: Fundamental experiments using the MRLS involved both liquid and solid samples at stand-off distances ranging from of 3 to 30 meters. All of the Raman spectra were corrected for dark current background and normalized for the transmission of the edge filter, the relative throughput of the spectrometer, and the channel-to-channel response of the detector.

ACCOMPLISHMENTS:

Work conducted during this fiscal year augmented DOE/NN-sponsored work on the Mini-Raman Lidar system by conducting much needed fundamental science on this new chemical sensor. Specifically the LDRD work focused on developing a better understanding of the performance issues associated with short-range, non-contact detection and identification of surface contamination.

- Detection of a 90-micron film of acetonitrile at 3-meters
- Detection of bulk materials at 30 meters
- Sensitivity: 0.25 gm/m^2 (1-sec int., 3-m)
- Detection of a VX surrogate (binary nerve agent) on various surfaces

PAPERS/JOURNALS/PUBLICATIONS:

1. Mark D. Ray and Arthur J. Sedlacek, "*Mini-Raman Sensor for the Remote, Stand-off Sensing of Chemical/Biological Substances and Method for Sensing Same*", U.S. Patent Pending (submitted 11/98)

2. Mark D. Ray, Arthur J. Sedlacek, and Ming Wu; *UltraViolet Mini-Raman Lidar for Stand-off, In-Situ Identification of Chemical Surface Contamination*, -- Rev. of Sci. Instrum *(in press).*

LDRD FUNDING:

FY 97	$ 99,066
FY 98	$ 99,778
FY 99	$ 93,980

Center for Imaging in Drug Abuse Research

Nora D. Volkow *97-68*

PROJECT DESCRIPTION:

The objective of this project was to provide the infrastructure to develop the NIDA /DOE Imaging Center at BNL. In turn the resources of this Center will be dedicated to gaining the knowledge required to advance the prevention and treatment of addiction and alcoholism while taking advantage of the imaging resources at BNL i.e. PET, SPECT and MRI.

TECHNICAL PROGRESS AND RESULTS – Fiscal Years 1998-1999:

The effort for this LDRD has been to initiate clinical studies with the MRI and to evaluate the potential of imaging technologies to detect disruption of the Blood Brain Barrier. The MRI studies required that we develop the programs that enable to acquire either relaxographic or spectroscopic information. The results from these efforts are summarized below. The scientists involved with these MRI studies include: J.S. Fowler, Y.-S. Ding, D. Franceschi, J.S. Gatley, H. Hetherington, J.-H. Lee, X. Li, P. Molina, J. Pan, W.D. Rooney, M Sammi, D. Schuhlein, F. Telang, N.D. Volkow, G.-J. Wang, C.S. Springer, Jr.

Spectroscopic Studies (Hetherington P.I.)

Purpose: One of the mechanisms by which alcohol conveys its intoxicating effects is hypothesized to be through its interaction with membrane lipids. As such the NMR visibility of alcohol in the human brain and its relationship to the pharmacological effects of alcohol have been an area of considerable interest. It has been reported that the visibility of brain alcohol is increased in alcohol tolerant subjects in comparison to non-tolerant subjects. Additionally, the effects of acute tolerance to alcohol consumption have been correlated with increased alcohol visibility in a two-drink paradigm. Despite these initial investigations of the effects of alcohol and NMR visibility, measures of the visibility of alcohol in the in vivo brain have varied widely ranging from 21% to 100%, depending upon the NMR acquisition method used. To date, with the exception of one study carried out in three volunteers, these studies have used single voxel measurements and have acquired little or no kinetic data. We therefore have focused our efforts on: 1) developing an in vivo NMR imaging method which minimizes artifacts and can be used in a kinetic mode (10 minute time resolution); and 2) have using this method to evaluate the regional kinetics of ethanol uptake and visibility in human brain.

Approach: We have studied seven individuals who received 0.5g/kg of ethanol while in the magnet. Spectroscopic images of alcohol content and measurements of venous blood alcohol levels were obtained both before drinking, and at ten-minute intervals after drinking for 90 minutes. Due to the predominant partitioning of alcohol to aqueous compartments, and differences in water content between white matter (WM), gray matter (GM) and cerebral spinal fluid (CSF), the tissue content of each spectroscopic imaging voxel was determined using a quantitative T1 imaging method.
Technical Progress and Results: In contrast to previous reports NMR studies, but in agreement with animal data, the brain alcohol concentration exceeded the blood level during the first thirty minutes after drinking. Using the final three time points,

when the absorption phase has concluded and venous blood levels are in near equilibrium with arterial and brain levels, the visibility was measured to be 1.00 ±0.20. These initial studies indicate that contrary to previous NMR studies, brain alcohol is 100% visible. This suggests that the previously reported alterations in visibility are most likely due to pulse sequence artifacts and changes in relaxation effects in detectable ethanol pools.

The results from this study are currently in press (Hetherington, H.P.; Telang, F.; Pan, J.W.; Sammi, M.; Schuhlein, D.; Molina, P.; and Volkow, N.D. Measurements of Human Brain Ethanol T2 by Spectroscopic Imaging at 4 T. *Magnetic Resonance in Medicine* (in press)) and we have submitted an NIH grant to continue this work.

Long-Term Objectives: We want to apply this methodology to investigate if there are differences in alcohol bioavailabilty between the genders that could help clarify the allegedly high susceptibility for the higher toxicity of alcohol effects in females than in males. We want to also apply the methodology to investigate the effects of repeated alcohol administration on the pharmacokinetics of alcohol in brain.

Relaxographic Studies (Rooney P.I.)

Purpose: Previous studies have reported that brain water proton T_1 values are decreased during acute ethanol intoxication. This is a potentially important observation since it could indicate that either brain water content decreases during acute ethanol intoxication, or that ethanol interacts with brain macromolecules to catalyze water proton T_1 relaxation. Previous studies have not examined the regional distribution of changes in water proton T_1. If they exist, regional T_1 changes could be important in elucidating details of ethanol's mechanism of action in the central nervous system. We therefore have focused our efforts 1) to determine the spatial distribution of changes in brain water proton T_1 values during acute ethanol intoxication, and 2) to establish the reproducibility of T_1 measurements in normal human brain at 4T.

Approach: We have studied five subjects who were scanned with the MRI in four different sessions: a) baseline (day 1), b) pre-EtOH (day 2), c) EtOH (day 2), and d) 24 hr post-EtOH (day 3). The EtOH session was started 60 minutes after drinking 0.75g/kg ethanol. During each MRI session a 3D anatomical image set with full brain coverage and a T_1 relaxographic imaging set from a single para-axial plane were acquired. Sixty-four images were collected at times that ranged from 0.027 to 17.1 sec following a non-selective adiabatic inversion pulse. Water proton T_1 maps were synthesized using the equation, $S(\tau) = S(\tau = \infty)[1-\beta \bullet \exp(-R_1\tau)]$; where, $S(\tau)$ is the measured pixel signal MRI intensity for inversion time τ, $S(\tau = \infty)$ is the steady-state value of the pixel MRI signal intensity, β relates to the efficiency of inversion, and R_1 $(=1/T_1)$ is the longitudinal relaxation rate constant. The T_1 maps had in-plane and through-plane resolutions of 3.5 mm and 10 mm, respectively. Regions-of-interest (ROIs) were manually selected from 12 bilateral brain areas; 1) peri-ventricular white matter, 2) frontal white matter, 3) thalamus, 4) caudate, 5) cortical-occipital gray matter, and 6) cerebral spinal fluid (CSF). T_1 values extracted from the ROI analysis were analyzed using a paired t-test. The reproducibility of the T_1 measurement was estimated from the baseline and pre-EtOH MRI sessions.

Results: Means and standard errors of water proton T_1 values for the six brain regions were found to be; 1) peri-ventricular white matter (890 ±11 msec), 2) frontal white matter (868 ±16 msec), 3) thalamus (1145 ±16 msec), 4) putamen (1180 ±25 msec), 5) cortical-occipital gray matter (1348 ±39 msec), and 6) CSF (3100 ±175 msec). There was no significant difference in water T_1 values for any of the MRI sessions or for any brain region. The T_1 reproducibility was excellent (95% confidence intervals were; precision: 0.959 • 0.057, accuracy: 0.998 • 0.003, and concordance: 0.951 • 0.051). These results indicate that at the moderate level of brain ethanol studied in this project, water proton T_1 values were not changed by more than 17 msec (1.8% relative) in white matter structures, and 45 msec (3.8% relative) in gray matter structures.

The results from this study have been submitted for publication and are under review (Rooney, W.D.; Lee, L.-H.; Wang, G.-J.; Franceschi, D.; Springer, C.S.; Volkow, N.D. 4.0 T Water Proton T1 relaxation times in normal human brain during acute ethanol intoxication. *Alc Clinical Exp Research* (submitted)).

Imaging Studies of the Blood Brain Barrier (Telang P.I.)

Purpose: Recent studies provided evidence that stress could disrupt the blood brain barrier and that this in turn would enable the passage of compounds that are normally kept outside of the brain. This was discussed in the context of Pyridostigmine, a carbamate acetylcholinesterase (AChE) inhibitor, which is used prophylactically against chemical warfare agents that does not cross the BBB. It was postulated that during stress this compound could penetrate into the brain and exert CNS effects. Furthermore it was hypothesized that the "central CNS " symptoms, (headaches, insomnia, drowsiness, nervousness, unfocused attention, and impaired capacity to conduct simple calculations) from soldiers during the Gulf War were due to entrance of Pyridostigmine into the brain.

Approach: To test if Pyridostigmine, could enter the brain during experimental stress we labeled it with C-11 and measure its uptake in control and in stressed rats (Swiss-Webster). The stress test used was the forced swimming test, which is a standard procedure for inducing stress responses in rodents. Pyridostigmine, was labeled with C-11 in the methyl group of the quaternary nitrogen atom, by reaction of $[^{11}C]$-CH_3I with desmethylpyridostigmine. The stress protocol involved two separate 4-minute periods of forced swimming in water at 21 ° C in a 3-liter graduated cylinder with a 4-minute rest period in between the swim sessions. The second swim session was followed by a 10-minute rest period and then immediately by a tail vein injection of 1 • Ci. of $[^{11}C]$-pyridostigmine. Animals were sacrificed 10 minutes later and whole brain, the head (skull), tail, and sample of whole blood from each mouse were placed individually in scintillation vials and counted in a Gamma Counter (Packard, MINAXI 5000 series.

Results: Contrary to expectations, stressed mice exhibited a slightly lower brain radioactivity than controls, possibly due to decreases in blood volume and brain interstitial fluid associated with hypercapnia from the stressful exercise. However, the decrease was not significant. The brain/ blood ratios for C-11 (0.035) were consistent with the tracer being confined to blood vessels, which account for up to 4% of total brain volume. The results from this

study have been published (Telang, F.W.; Ding, Y.-S.; Volkow, N.D.; Molina, P.E.; and Gatley, J.S. Pyridostigmine, a carbamate acetylcholinesterase AChE inhibitor and reactivator, is used prophylactically against chemical warfare agents. *Nucl Med Biol* **26,** 249-250, 1999).

Long-Term Objectives: We will not continue these studies since they did not show evidence of BBB disruption with stress. However, we will continue to develop PET ligands like Pyrodistigmine that may be beneficial in detecting BBB disruption on other conditions (i.e multiple sclerosis, radiation into the brain). We have started studies to investigate the usefulness of iron nanoparticles to measure BBB disruption with the 4 T MRI.

Imaging studies to evaluate the cerebral circulation in substance abusers

Purpose: PET imaging studies have given evidence of marked disruptions in cerebral blood flow in chronic cocaine abusers. Moreover clinical studies documenting strokes after cocaine have provided direct evidence of the deleterious effects of cocaine to the cerebral circulation. The purpose of these studies was to take advantage of MRI to investigate the cerebral circulation in chronic cocaine abusers.

Approach: We have used two strategies to investigate cerebral circulation in cocaine abusers, one is to measure the responsivity of cerebral blood vessel to external stimulation using fMRI (Telang and Wei Lee P.I) and the other was to assess changes in blood brain barrier permeability using gadalinium and MRI (Rooney P.I). The fMRI capitalize on the fact that the activation signal requires the increase in cerebral blood flow to the area that is activated. We postulated that in cocaine abusers this signal would be blunted as a result of compromise of the blood vessels. We have studied 10 cocaine abusers and 5 controls with fMRI to measure the activation of the visual cortex to a strobe light of different frequencies.

For the BBB studies we postulated that cocaine abusers would have changes in BBB permeability which would lead to an abnormal accumulation of gadolineum within the brain tissue.

Results: Preliminary analysis of the functional activation studies revealed that contrary to our hypothesis cocaine abusers showed an enhanced response to visual stimulation when compared with controls. This enhanced response was reflected both as an increase in the signal intensity as well as an increase in the volume that showed an activation signal. We have interpreted these results as reflecting either a hyper-excitability of the brain tissue secondary to cocaine discontinuation or as an inadequate efficiency of the brain that requires commitment of larger volumes of tissue to execute a given function.

Preliminary analysis of the data on BBB in the cocaine abusers revealed that contrary to our hypothesis these subjects showed a reduced accumulation of the gadolinium when compared with controls. We believe this reflects either a decrease in cerebral blood flow, which results in decreased delivery of the contrast agent or a disruption of the permeability of the contrast agent through the BBB.

Long-Term Objectives: We plan to use these data to request funding from NIH to investigate if the changes in activation in the cocaine abusers are a function of excitability of cerebral inefficiency and to assess if they

recover with detoxification. We plan to also request for NIH funding to further characterize the extent to which the BBB is impaired by coupling the MRI studies with PET studies with radiotracer to assess BBB permeability.

PAPERS/JOURNALS/PUBLICATIONS:

Hetherington, H.P.; Telang, F.; Pan, J.W.; Sammi, M.; Schuhlein, D.; Molina, P.; and Volkow, N.D. Measurements of human brain ethanol T2 by spectroscopic imaging at 4 T. *Magnetic Resonance in Medicine* 42:1019-1026, 1999

Rooney, W.D.; Lee, L.-H.; Wang, G.-J.; Franceschi, D; Springer, C.S.; Volkow, N.D. 4.0 T Water Proton T1 relaxation times in normal human brain during acute ethanol intoxication. *Alc Clinical Exp Research* (submitted). 2

Nora D. Volkow, Gene-Jack Wang, Joanna S. Fowler, Dinko Franceschi, Laurence Maynard, Christopher C. Wong, Christoph Felder, Jing-Huei Lee, William D. Rooney, Jullie W. Pan, Naomi R. Pappas, and Charles S. Springer. Resting brain metabolic activity when subjects are exposed to a 4 Tesla magnetic field. (in preparation)

FOLLOW-ON FUNDING:

See each individual project for future funding plans.

LDRD FUNDING:

FY 1998	$332,826
FY 1999	$341,508

Performance Enhancement in a Photoinjector Electron Linac

Erik D. Johnson *98-23A*
Louis F. DiMauro
William S. Graves
Brian Sheehy and
Xijie Wang

PROJECT DESCRIPTION:

This work explores previously unmapped parameter space in Photoinjector Electron Linacs with the goal of finding approaches to dramatically improve the performance of this class of machines. There are conflicting theoretical predictions of performance particularly when short and shaped laser pulses are used for driving the photocathode. Some project dramatic enhancement, some marginal improvement, and at present no data exist to sort them out. At a minimum this work represents an experimental investigation to corroborate theory; if successful it provides a proof of principle for a significantly improved performance electron machine.

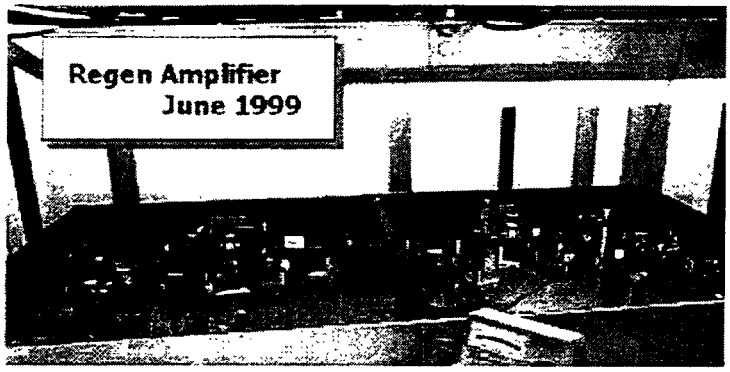
APPROACH:

In previous supported activities at BNL, the Accelerator Test Facility developed an RF photo-cathode gun that was the starting model for our gun (Gun IV). Our gun can be run at higher repetition rate (due to enhanced cooling). To allow better control of the temporal characteristics of the light used to stimulate emission from the cathode, we have developed a laser system using Titanium Sapphire technology, which provides superior bandwidth to allow pulse shaping.

PROGRESS:

We have assembled the requisite laser components, and developed an adjustable harmonic generator to make 266 nm light (using BBO). We opted to configure the gun and laser to allow normal incidence illumination of the cathode, which simplifies the manipulation of the wave front to assure a narrow arrival time at the cathode surface. Both the ATF and LEAF facilities use grazing incidence to enhance photo-yield, with the penalty of more difficult wave front correction optics. Measurements are underway to optimize focal properties (transverse profile), pulse distribution (length and longitudinal structure), and phasing with respect to the photo-injector RF.

Laser System installed at SDL. Titanium Sapphire Oscillator is in the foreground, the Nd:YAG pump lasers at the right. The amplifiers are the background. Dedicated diagnostics are installed to monitor performance during operation.



Laser System amplifier. It is a three stage system with a seeded regenerative amplifier followed by two double pass amplifiers, one of which can be bypassed when only gun operation is required. The additional IR beam power will be used for driving beam diagnostics, and generating seed radiation.

ACCOMPLISHMENTS:

The laser system is performing above specification in the IR. An achromatic transport system has been installed and beam successfully transported from the laser to the photo-injector. Pointing and timing stability measurements thus far have shown adequate performance. During FY 1999 we obtained permission to run RF tests and condition the linac pending a full ARR.

PAPERS/JOURNALS/PUBLICATIONS:

[1] "The Deep Ultra-Violet FEL", E.D. Johnson, Presented at FEL 99 Conference, Hamburg Germany, August 23-27 1999.

LDRD FUNDING:

FY 1999	$300,339
FY 2000 (estimate)	$266,000

Pulse Compression and Emittance Preservation in a High Brightness Electron Linac

William S. Graves 98-23B
Richard Heese
Erik D. Johnson

PROJECT DESCRIPTION:

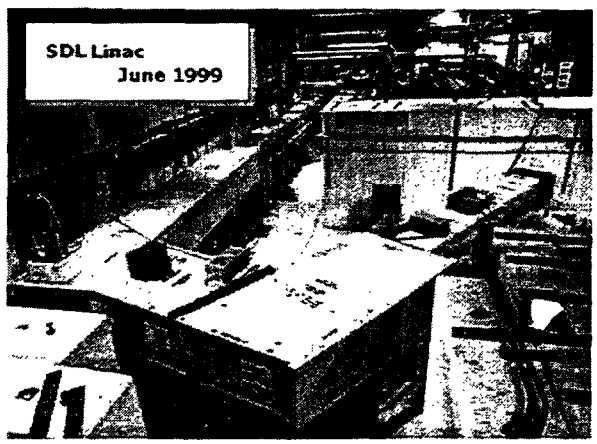
For Free Electron Lasers substantial performance gains could be obtained if peak current in electron linacs can be increased. This outcome might be achieved by compressing the longitudinal extent of the electron bunch, but it is only beneficial if the properties of the beam are not degraded. Substantial emittance growth due to the pulse compression process has been theoretically predicted, although extant theories vary by more than an order of magnitude in the estimates of the effect. By an experimental study, we can quantify the effects and investigate some of the proposed schemes to mitigate the emittance dilution induced by Coherent Synchrotron Radiation production and Coherent Space Charge Force interactions with the electron beam. If successful, this project may help define the practical limits for the use of pulse compression in advanced machines.

APPROACH:

We have developed strategies to meet the stringent requirements for the production and preservation of bright electron beams within the framework of existing hardware that can support our experiments. Although there are many aspects to the undertaking, a key element of our approach has been the development of a magnetic pulse compression system. A second element of our approach has been to develop suitable diagnostics for verifying the properties of the electron beam produced.

PROGRESS:

We have reconfigured the 230 MeV SXLS (Superconducting X-ray Lithography Source) linac to be used for these experiments. Working from the established baseline parameters for our accelerator, we have developed some of the tools for high brightness electron beam preparation and measurement. To the extent possible, we have prepared and qualified these tools. Full testing awaits approval of operations for the SDL (Source Development Laboratory, Building 729). Diagnostics for determining position and size of the electron pulse were prototyped and developed for installation in 22 locations on the linac so the beam properties can be evaluated all the way through the machine.



SDL Linac as mechanical reinstallation was nearing completion. The enclosure around the linac is precast lead shielding, a minimum of two inches in thickness.

ACCOMPLISHMENTS:

During FY 1999 we obtained permission to run RF tests and condition the linac pending a

full ARR (Accelerator Readiness Review). We installed the required shielding, security systems, and equipment controls to operate the linac. We have installed the pulse compressor and performed the first commissioning measurements. Although the conditioning operations protocol does not allow us to run with photocurrent the data obtained from dark current produced during testing are encouraging. The compressor is functional and operates as expected although full testing is not possible until operations with photocurrent are approved (anticipated January 2000). Steering errors have been very small and so far readily corrected. Installation of the synchrotron radiation diagnostic is underway. The monitor systems have already proven useful in steering the dark current and phasing the linac sections with respect to each other. Without feed back, RF stability the order of 2 degrees or better from one system to the next has been obtained.

PAPERS/JOURNALS/PUBLICATIONS:

[1] "Design of the Source Development Lab Bunch Compressor," W.S. Graves, I. Ben-Zvi, E.D. Johnson, S. Krinsky, J. Skartika, M.H. Woodle, L.-H. Yu, and T.O. Raubenheimer, IEEE Particle Accelerator Conference, 1997.

[2] "A High Resolution Electron Beam Profile Monitor and its Applications," W.S. Graves, E.D. Johnson, S. Ulc, 1998 Beam Instrumentation Workshop, AIP Conference Proceedings Vol 451 p. 206, (1998)

[3] "Periscope Pop-in Beam Monitor," E.D. Johnson, W.S. Graves, and K.E. Robinson, 1998 Beam Instrumentation Workshop, AIP Conference Proceedings Vol 451 p. 479,(1998)

[4] "The Deep Ultra-Violet FEL," E.D. Johnson, Presented at FEL 99 Conference, Hamburg Germany, August 23-27 1999.

LDRD FUNDING:

FY 1999	$150,621
FY 2000 (estimate)	$134,000

Novel Mechanisms of Hydroxy Fatty Acid Biosynthesis

John Shanklin *98-27*

PROJECT DESCRIPTION:

Plant fatty acids represent an $80 billion dollar a year market. However, the fatty acid compositions of crop plants contain a relatively small diversity of compared to the diversity found in nature. A goal of this laboratory is to increase this diversity. Crop plants vary in their fatty acid composition in terms of the degree of desaturation and in the chain length of the fatty acids. There are uncommon plants with unusual fatty acids such as hydroxy- and epoxy groups. These fatty acids are desirable because the functional groups are stereospecific and can be easily derivitized and therefore used for specific industrial starting materials such as lubricants and plasticizers which are currently obtained from petrochemicals. Much of the work in this laboratory has focussed on oxygen-dependent lipid modification enzymes that use diiron clusters for catalysis. While these systems constitute by far the most widespread class of lipid modification enzymes, there also exist a class of anaerobic enzymes that perform hydroxylation. The differences between these enzymes are that the aerobic class attack a saturated portion of the acyl chain, whereas the anaerobic hydroxylases hydrate an existing double bond.

Anaerobic hydroxylases or olefinic hydratases are found in both higher plants and in bacteria. Our goal is to clone the gene(s) encoding the hydratase and explore the possibility of using the system to modify plants to produce hydroxylated fatty acids via the anaerobic pathway.

TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

Purpose: The purpose of this research is to define alternate metabolic pathways for the production of hydroxy fatty acids in plant seed oils. Objectives to be achieved include: Identification of appropriate organisms that use anaerobic hydroxylases, isolation of the anaerobic hydroxylases enzyme, isolation of the anaerobic hydroxylases gene, biochemical characterization of the recombinant enzyme, and construction and evaluation of stable transgenic plants.

Approach: Several approaches were initiated, one using plants as a source of material, the other using bacteria.

For the plant approach we identified the indrajao, or *Wrightia tinctora* as a seed with approximately 60% isoricinoleic acid. Previous studies by others showed that developing seeds could synthesize 18:1 9-OH anaerobically. Our intent was to grow the plant and to harvest seed and use a conventional protein purification and enzyme assay analysis. For the bacterial approach, we undertook a genetic approach to directly identify the gene of interest. The idea was to identify species of bacteria that are related to *E. coli* such that expression of their genomic DNA would result in the accumulation of active anaerobic hydroxylase. This we could then assay if we could develop an assay to detect the hydroxylated reaction product.

Status: 1) Plants. We identified a seed source for plants that contain isoricinoleic acid, and purchased several pounds of indrajao seeds. Unfortunately the plants are rather slow growers and we are still waiting for them to set seed that we can use as source material for the isolation of enzyme.

2) Bacteria. We successfully developed a visual screening technique that allows us to identify bioconversion in a mass format using ether extractions of the culture media that had been spiked with oleic acid and incubated for several days. The assay was verified using thin layer chromatography and gas chromatography/mass spectrometry. Many bacterial species that had been reported to perform the bioconversion of oleic to hydroxystearic acid were screened and it was confirmed that most of them indeed perform this function.

We identified *Micrococcus leuteus* as a microbe that both constitutively expresses a hydratase and is amenable to the technical manipulations required to extract protein and DNA. Thus, we isolated *M. leuteus* genomic DNA and constructed a library consisting 1000 clones (5 genome equivalents) that should in theory give a 98+% chance of identifying any particular gene. This library was introduced into *E. coli* which lack the constitutive hydratase activity, and the resulting clones were screened for bioconversion of oleate to 10-hydroxystearate. We made an important finding, that many of the colonies (approximately 10%) were giving positive results. This figure is too high because we expect perhaps 0.1-0.5% positives. This prompted us to investigate *E. coli* more deeply. This investigation revealed that while *E. coli* lacks a constitutive oleate hydratase activity, it contains an inducible one for which we have subsequently defined the appropriate inducting conditions. This is actually an ideal situation because the powerful genomic and proteomic tools become available to help identify the genetic basis for this activity. Thus, we have returned to the direct approach of protein purification. We have been successful in using differential ammonium sulfate precipitation, and the following HPLC chromatographic steps: phenyl sepharose, Q-anion exchange chromatography, and preparative size exclusion methodology. We are currently in the process of defining which band the protein represents by poly acrylamide gel electrophoresis.

Future Work: Once candidate bands are identified, we will ship a sample of candidate bands for mass spectral investigation at the Yale center for macromolecular studies. By specific digestion of the contents of this band and mass determination of the fragments, the protein will be identified by matching the fragment profile with a library containing the entire predicted fragment patterns for the entire *E. coli* genome. Once identified the open reading frame corresponding to the gene will be tailored for expression in the T7 expression system for the production of large amounts of protein. The protein will be purified to homogeneity, biochemically characterized. At the same transformation vector suitable for *Agrobacterium* and introduced into *Arabidopsis thaliana* under the control of a strong seed specific promoter. The composition of seed fatty acids will be compared to that of controls containing a blank plasmid.

FOLLOW-ON FUNDING:

A multi-year CRADA with The Dow Chemical Company and Dow Agrosciences will be based on this research. The Office of Technology Transfer is in the process of finalizing the agreement.

LDRD FUNDING:

FY 1998	$99,646
FY 1999	$101,881

Sensitive Detection and Rapid Identification of Biological Agents by Single Molecule Detection

Ming Wu *98-58*

PROJECT DESCRIPTION:

The objective of this LDRD is to integrate the techniques of fluorescence immuno-assays, capillary electrophoresis (CE), and single-molecule detection (SMD) into a single compact instrument for the rapid and reliable identification of biological agents. An integrated instrument based on these techniques is expected to be capable of analyzing as few as 100 tagged biological agents in *micro*-liter samples within minutes. The proposed analytical system has uses in the areas of BW-related agent detection, environmental monitoring, and medical testing.

TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

Purpose: The *rapid detection and reliable identification* of biological agents is of utmost importance to those concerned with BW-related agent detection, public health, and environmental protection. Our goal is to develop a sensor, which can identify a small number of biological agents with high selectivity, sensitivity, and negligible false positives and false negatives.

Approach: Experimental procedures for identification include: (1) incubation of a sample containing suspect antigens with the fluorescence-labeled antibodies; (2) injection of the sample into a capillary tube for separation by the capillary electrophoresis; and (3) detection of the individual fluorescence labeled antibody-antigen complexes in a micro-flow cytometer by single-molecule detection using laser-induced fluorescence. The selective nature of antibody binding provides a highly accurate means of identification of target biological agents. The highly selective bindings of antibodies are used to attach fluorescent tags. Capillary electrophoresis is then used to rapidly separate the fluorescence labeled antibody-antigen complexes from the unbound antibodies and other components of the complex mixture. This separation is critical in reducing or even eliminating false-positive identifications in the detection of the biological agents. The separated samples in the capillary are placed in the micro-flow cytometer. Laser-based optical techniques capable of single molecule detection are used to detect the fluorescent tags.

Technical Progress and Results:

A micro flow cytometer was built and computer software was developed for SMD experiments. The performance of the system was examined by DNA fragment sizing of the λ DNA/Hind III fragments stained by POPO-3 dye. The agreement between the measured and calculated transit time implies that our apparatus was detecting single molecule events. The burst size versus DNA fragment length is demonstrated to have a linear relationship, as expected. The apparatus is capable of detecting single fluorescence labeled antibodies and antibody-antigen complexes. We have demonstrated the viability of single molecule detection for fluorescent-labeled antibodies, such as R-phycoerythrin goat anti-rabbit IgG(H+L) conjugate in flow. B-phycoerythrin conjugates, anti-mouse IgG,

$F(ab')_2$ fragment specific was used as a fluorescent labeled antibody, and anti-human IgG (H+L), $F(ab')_2$ was selected as the antigen. Figure 1 shows the detection of single immuno complexes in the flow. It is interesting to note that the photophysical properties of the selected fluorophores have not changed significantly when bound to the antibodies and to the immuno complexes. A capillary electrophoresis system was integrated with the single molecule detection system. Figure 2 shows the electropherograms of B-phycoerythrin labeled IgG $F(ab')_2$ and its immuno complexes. This immunoassay seems not to have adsorption problems under current conditions. There are no tailings in the electropherograms for both the free B-phycoerythrin labeled antibody and the immuno complexes. It should be pointed out that the mobilization time of the complexes is shorter than the free B-phycoerythrin labeled antibody. This agrees with immunoassays reported in the literature. This important property will prevent potential problems in the trace detection of antigens due to high concentrations of free fluorophore labeled antibodies in the solutions.

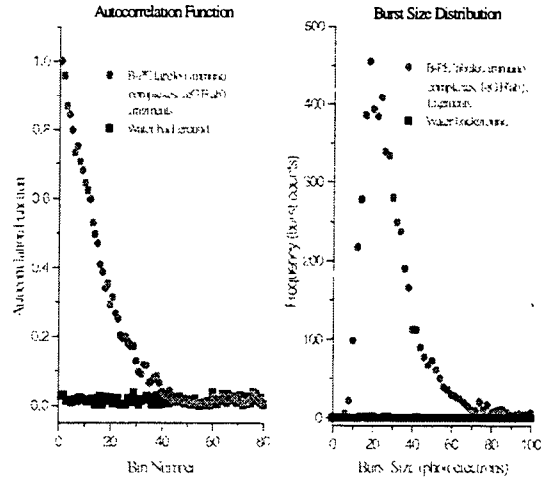


Figure 1. Detection of single immuno complexes, B-phycoerythrin labeled IgG $F(ab')_2$ fragments.

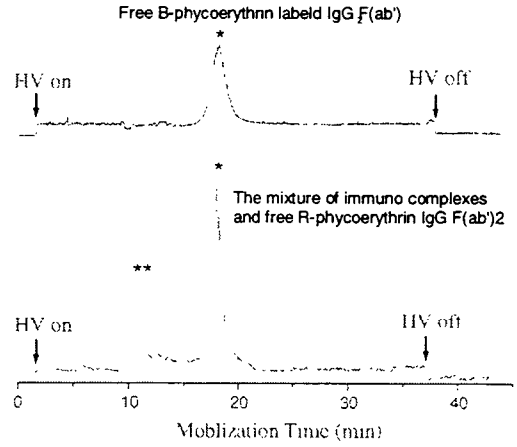


Figure 2. Electropherograms of B-phycoerythrin labeled IgG $F(ab')_2$ and its immuno complexes. The capillary electro-phoresis was preformed in a 35-cm long, 20 μm I.D. and 90 μm O.D. bare capillary. The buffer solution inside of the capillary was 1X TBE (PH = 8.4), and the buffer solution in the sheath flow was X TBE. Applied voltage was 5 KV. The * indicates free B-phycoerythrin labeled IgG $F(ab')_2$ fragments, and the ** indicates the immuno complexes of IgG $F(ab')_2$ fragments.

ACCOMPLISHMENTS:

A core competence has been established in single molecule detection and its applications under this LDRD. The successes of the proof-of-principle experiments provide a scientific basis for potential solicitation of external funding. During past two years, proposals were submitted to ERDEC, US Army and CBNP, DOE. A manuscript describing the results is under preparation for publication.

LDRD FUNDING:

FY 1998	$100,787
FY 1999	$ 99,618

Ultra-Fast Detector Based on Optical Techniques

Yannis K. Semertzidis *99-01*

PROJECT DESCRIPTION:

Statement of Work: The purpose of this LDRD was to develop the first, electro-optical (e-o) charged particle detector based on the Pockels effect. Since this technique is sensitive to the presence of electric fields rather than charge collection, the inherent resolving time is not limited by electron mobility or detector capacitance. The intrinsic time limitation is in the femtosecond (fs) time scales and can sense the charged particles in a non-destructive way.

The electric field from a charged particle beam influences the electrons of a dielectric material located near the charged particle beam path. A polarized laser light traveling in the dielectric material (e.g. $LiNbO_3$ an electro-optic crystal) senses this influence within a time scale determined by the laser wavelength, i.e. of order of a few fs depending on the laser wavelength. The duration of the electric field, for a relativistic beam, is equal to the beam bunch due to Lorentz field contraction. It is, therefore, very attractive to use this technique for beam diagnostics in accelerator development. Other uses include the application of the method as a readout of a particle detector offering high rate capability and high sensitivity.

APPROACH:

Our experience with lasers, polarimeters, and ellipsometers together with our background in particle and accelerator physics has led us to propose this experiment. Sensing of ultra-fast electric fields with e-o techniques based on the Pockels effect have been reported before in the literature. We brought this technique and applied it to accelerator and particle physics. The question was whether the expected small size signal would be possible to detect in such a noisy environment.

In order to test the feasibility of this idea, we went to the Accelerator Test Facility (ATF) of BNL where a pulsed electron beam is available at 1.5Hz rep-rate. We used a polarization maintaining (PM) fiber to bring a polarized laser light into a vacuum chamber. There the light is coupled to an e-o crystal ($LiNbO_3$) and next via another PM fiber is carried outside the beam vacuum tube for analysis. A quarter wave plate and an analyzer (forming an ellipsometer) is used to analyze it. A fast detection system is used at the end to provide the signal for further processing.

This is an effort of 11 physicists from BNL, Montclair State University and the University of Pittsburgh, with experience in Particle, Accelerator, and Laser Physics.

TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

In 1999 we have established for the first time in the world that it is possible to observe the charged particle beam in a non-destructive way using e-o techniques.

We have used the electron beam from the ATF with a total charge of about 1nC per bunch, and 10ps total bunch length focused to 1mm diameter. The energy of the electrons was 45MeV. Our crystal was located approximately 1cm away from the beam path. The charged particle beam creates an electric field (E) which produces,

in the e-o crystal, an ellipticity of approximately $\vartheta = 10\text{mrad}$ for 10^{10} electrons in the beam. The signal-to-noise ratio (SNR) for a detection system which is photon statistics limited is given by

$$SNR = \vartheta\sqrt{\frac{PTq_p}{2\hbar\omega}}$$

with P the laser power, T the inverse of the detection system bandwidth, q_p the quantum efficiency of the photodiode, and $\hbar\omega$ the energy of the laser photon. As an example we will take an electron particle beam with T=10ps, q_p = 0.8, P = 1mW, for N_e= 10^{10}, and $\hbar\omega$ = 0.9eV, then SNR = 1.7. At the experimental setup we used a CW laser of 10mW, and a detector with 100ps time

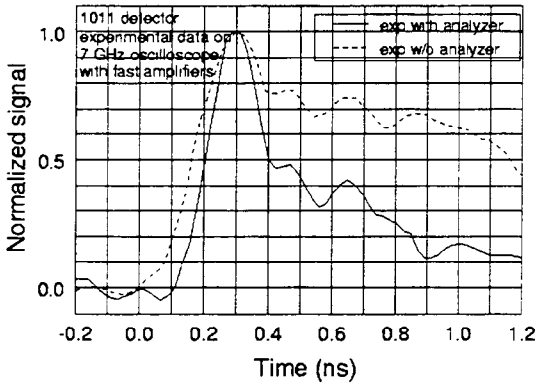


Figure 1. The polarization dependent (solid line) and polarization independent (dash line) signal.

In Figure 1 we show the polarization dependent signal (solid line) as observed with a single shot of the electron beam. The maximum modulation of the light intensity was about 9% of its DC level.

We have also observed a signal when the crystal intercepted the beam which is shown in Figure 1 again in the single shot mode (dash line). We repeated this without the analyzer present and found it was independent of it. The difference from the polarization dependent signal is two-fold. First it does not flip sign under any polarization orientation, and second it has a much longer time decay constant.

So far we have used the fastest photo-diodes, amplifiers, and oscilloscopes available to us to detect those signals. The real benefit of the technique, however, is only possible to achieve when purely optical techniques are used because of their much greater bandwidth capability and it is our goal for the FY2000.

ACCOMPLISHMENTS:

The results were presented (oral presentations in both cases) at the Particle Accelerator Conference of 1999 held in New York City (March 29th-April 2nd, 1999) by Yannis Semertzidis and at the International Europhysics Conference-HEP99 held in Tampere, Finland by Don Lazarus. In both occasions the interest of the audience was great since this is the first observation of a charged particle beam via the electro-optic technique. We are in the process of writing a NIM article. There is a graduate student (Dimitrios Nikas from the University of Thessaloniki/Greece) who is entirely supported by this LDRD.

LDRD FUNDING:

FY 1999	$113,345
FY 2000 (estimate)	$ 90,000

Nova: Networked Object-based enVironment for Analysis

Torre Wenaus *99-03*
Tim Hallman
Sasha Vanyashin

PROJECT DESCRIPTION:

The LDRD work "Proposal to Develop A State of the Art Object Oriented Analysis Framework" was initiated last year to draw on RHIC software experience for the development of generic analysis tools which can be widely applied within and beyond High Energy and Nuclear Physics (HENP), with particular focus on distributed computing. The aims of this project are being realized in the development of NOVA, a Networked Object-based enVironment for Analysis that employs the burgeoning technologies of the internet to provide generic distributed Object Oriented (OO) analysis tools. Our strong reliance on internet-driven open software technologies differs substantially from the in-house or commercially developed solutions current in the field, but offers large potential benefits in exploiting this area's exponential growth. If the approach succeeds and these technologies can be adapted to distributed physics analysis, the work will demonstrate the low manpower cost and high levels of functionality offered by our approach. The project has already established a recognized distributed analysis expertise at BNL that has led to a US ATLAS Computing funding proposal in this area and has garnered wider interest in the community.

APPROACH:

experiments already have established OO frameworks in production or under development. frameworks are weak in their support for distributed analysis in large, geographically dispersed collaborations. The NOVA project does not reinvent or evolve existing analysis frameworks, but rather provides new functionality via modular components providing application-neutral interfaces that can be used in isolation to extend the capability of existing analysis systems.

NOVA architecture components are distributed among the four principal domains of mobile analysis: client, central analysis server, middleware, and data management. A mobile analysis client interacts with a central analysis server and associated monitoring and control tools via web-based middleware to support analysis in a distributed heterogeneous environment. software distribution, management and version coordination tools to meet the collaborative analysis needs of a widely distributed community. Central data and file catalogues with associated tools for controlling and monitoring data locality, data browsing, and data model evolution for data intensive analysis are included. We focus on supporting C++, the most widely used OO language in HENP. NOVA is being developed using an iterative process driven by user participation and closely coupled to prototyping in real-world experiments (STAR, ATLAS).

In evaluating and selecting technologies we have imposed the requirements that they should be free or nearly so to minimize buy-in cost, and should be widely used standards showing good support and strong growth. Following these requirements we have adopted many open software tools including the MySQL database, the Apache web server and associated integrated tools, XML based information exchange, and the ROOT object oriented toolkit for HENP analysis.

TECHNICAL PROGRESS:

In its first year the project has designed a distributed computing architecture and toolset that has captured interest and/or applications in RHIC and LHC experiments, including STAR, ATLAS and LHCb. All key components of the architecture have been prototyped or implemented, completing our year one schedule on target. Because NOVA developers are STAR and ATLAS collaborators these experiments have served as convenient test beds. The computing leadership of the LHCb experiment has visited BNL to learn about NOVA.

We have implemented distributed computing and analysis tools in the areas of configuration and parameter databases, file catalogs and event meta-data databases, web-based browsers and management tools, and communication and distributed development tools. We have implemented mobile analysis clients and a distributed analysis server system for job editing and submission, based on a centrally managed database and web-based clients. We have implemented a machine, user, job and data monitoring system that provides a unified view of analysis resources possibly spread across several sites. All these tools are deployed in production or prototype form within STAR, database tools are deployed in prototype form in ATLAS, and analysis monitoring tools are in production in US ATLAS. NOVA tools were successfully used for storage and object-based retrieval of the geometry parameters for the detector simulation of the ATLAS calorimeter.

In FY00 we will complete the implementation guided by application and prototyping in STAR, ATLAS, and potentially other environments, and establish NOVA as an experiment-independent tool set for distributed analysis. We will perform scalability testing with management of multi-terabyte data sets and large scale analysis.

ACCOMPLISHMENTS:

FY1999 NOVA results were presented to the HENP community at the Computing in High Energy Physics conference CHEP2000 in January 2000. A NOVA paper is included in the proceedings. Presentations on NOVA have been made to STAR, US ATLAS, International ATLAS and LHCb. NOVA was presented to the wider community at the "Open Source/Open Science 1999" conference at BNL. The NOVA project is presented on the World Wide Web at http://www.usatlas.bnl.gov/computing/nova. As a direct result of NOVA, funding from LBNL's HENP Grand Challenge (GC) project was obtained to support one of us (Sasha Vanyashin) in FY2000 to integrate GC with STAR software incorporating NOVA components. Future programmatic funding based on experience accumulated in NOVA is being sought in the developing Grid Computing initiatives of various agencies and in the core software project of US ATLAS.

LDRD FUNDING:

FY 1999	$99,894
FY 2000	$80,000

Aerosol Module for Climate Models Using Advanced Computer Techniques

Carmen M. Benkovitz *99-05*
Stephen E. Schwartz
Robert L. McGraw
Douglas L. Wright
Hong Ma
Arnold M. Peskin

PROJECT DESCRIPTION:

Technical Objective: Given the necessity of including aerosols in climate models, methods must be developed that will allow aerosol chemical and microphysical processes to be accurately and efficiently represented in the next generation of climate models. The overall objective of this proposal is to develop computational techniques to include aerosol transport and evolution processes in climate models and thus position BNL as a major participant in research on aerosol influences on climate and regional scale air quality.

APPROACH

Background: We and others have presented a body of work over the past decade that indicates that anthropogenic aerosols are exerting an influence on climate change that is comparable (but of opposite sign) to the anthropogenic greenhouse effect. Aerosol chemistry must be included on-line in climate models in order to represent any feedbacks from local to global, caused for example by differential heating.

Methods: Our group at BNL has developed a hemispheric three-dimensional Eulerian transport and transformation model of the sulfur cycle the Global Chemistry Model driven by Observation-derived meteorology, GChM-O. The model has been expanded to include the treatment of aerosol microphysics using the Quadrature Method of Moments (QMOM) [*McGraw*, 1997; *McGraw et al.*, 1995a; *McGraw et al.*, 1995b] an accurate but computationally intensive methodology developed at BNL under NASA funding to represent aerosol properties important to their effect on the radiative balance of the Earth and thus on global climate.

TECHNICAL PROGRESS AND RESULTS:

The ability to represent aerosol microphysics in a sub-hemispheric scale transport and transformation model by the method of moments has been demonstrated [*Wright et al.*, 1999]. Aerosol optical and radiative properties have been calculated from the moments of the size distribution, thereby substantiating the utility of the moment approach for examining the influence of aerosols on climate [*Wright*, 2000]. The aerosol module code has been parallelized for more efficient calculations.

The sub-hemispheric chemical transport and transformation model had been previously expanded to hemispheric under DOE support. This version has now been parallelized. and is a host model for the parallelized aerosol module.

Computationally intensive, parallelized models on both the regional and global scales into which the moment representation of aerosol microphysics can be incorporated have been identified and collaborations with the principal designers of these models (D. Roberts, UK Meteorological Office for global scale model; J. Seinfeld, Caltech, and D. Dabdub, UC Irvine, for regional scale model) have been initiated.

S. Schwartz participated in preparation of a proposal to the National Science Foundation "Knowledge and Distributed Intelligence" Program entitled "Tools for the Analysis of Fluid Flow." The proposal was spearheaded by J. Glimm (SUNY, and now also BNL) and included participation from Los Alamos National Laboratory, Lawrence Livermore National Laboratory, BP Amoco, Chevron, University of Colorado, and Stanford University. Although the proposal was not successful, the effort expended in preparation of the proposal and the collaborations forged will place BNL in an enhanced position to secure funding in future opportunities.

SPECIFIC ACCOMPLISHMENTS

Wright, D.L., Retrieval of Optical Properties of Atmospheric Aerosols from Moments of the Particle Size Distribution, *J. Aerosol Sci.*, 31, 1-18, 1999.

Wright, D.L.; McGraw, R.; Benkovitz, C.M.; and Schwartz, S.E. Six-Moment Representation of Multiple Aerosol Populations in a Sub-Hemispheric Chemical Transformation Model, *Geophys Res. Lett., 27, 967-970* 2000.

Wright, D. L.; McGraw, R. L.; Benkovitz, C. M.; and Schwartz, S .E. Aerosol Dynamics and Shortwave Radiative Forcing in a Sub-hemispheric Model by the Method of Moments. American Geophysical Union 1999 Spring Meeting, Boston, MA, Jun 1-4, 1999; paper A22G-08. Abstract: *Eos, Trans. Amer. Geophys. Un.* **80** (No. 17, Supplement) S41 (1999).

Benkovitz, C.M. Preparing to Model the ACE Experimental Periods with GChM-O Version 2 and Recent Developments Regarding Aerosol-Related Emissions Inventories. Third Annual Workshop of the Northern Aerosol Regional Climate Modelling Project (NARCM), March 1-2, 1999, Toronto, Ontario, Canada.

LDRD FUNDING:

FY 1999	$98,887
FY 2000 (estimate)	$80,000

Environmental Carbon Observatory

George R. Hendrey *99-06*

PURPOSE:

The purpose of this work is to advance the conception of, and carry out preliminary technical analyses of experimental facilities and devices that would be required for a global-scale environmental research facility tentatively called the Environmental Carbon Observatory (ECO). The goal is to evaluate a coherent system for integrating environmental carbon cycle measurements and models. In particular, we will construct and evaluate the data acquisition, communications and management software applied to current Free-Air CO2 Enrichment (FACE) field sites as a model of an integrated ECO facility.

APPROACH: A meeting of experts was used to advance the concept of how to address the global carbon cycle, to refine scientific questions, and to outline innovative approaches to both the scientific and technical problems associated with quantifying terrestrial carbon flux on a global scale. Software will be developed in order to determine the utility of one of the ECO concepts, that data from highly dispersed sources can be made available in real-time via the internet, and stream directly to process-based models of carbon cycle components. Although it sounds a trivial issue, making software to fit experimental needs, that is readily accessible to the widest range of users, most of whom are not programmers, in a seamless and integrated way, is a serious technical issue and impediment to integrated science. Programs will be based on Microsoft Component Object Model (COM) technology using Visual Basic as a development platform. Software interfaces for data loggers, LAN and Internet-based communications will be built as a seamless system that allows data flow from the instrument to local site servers and automated uploads to Structured Query Language (SQL) database located at BNL. Report generators will be written that put near real-time data reports onto web sites that will be developed for participating projects. Remote users will have access to the data and reports through Open Database Connectivity (ODBC) to various on-line data products. It is the integration of these elements that is the difficult step.

TECHNICAL PROGRESS AND RESULTS:

A meeting of experts was held to study innovative approaches to scientific and technical problems associated with a facility of the scale of ECO. This resulted in a clear statement of the science questions that ECO would address and an outline of the approach to be followed in further development of the facility. Steven Humphries was hired and given a project appointment in order to begin the development of the needed software. He is working with members of the FACE project team to build and implement these capabilities at some of our field sites and to implement them on the Internet. FACE field facility sites are used as development platforms for ECO tools. The FACE home page (http://www.face.bnl.gov/) is now a rich source of information about the FACE project and more importantly for ECO is a host environment for the acquisition, management and display of diverse experimental data using the Internet.

The Data Manager section of our web site is our Internet gateway to this experimental

work. Here you will find online and downloadable data sources from the various participating sites, along with the latest tools for their analysis and management. With these pages you can:

- Examine near live data streaming from remote experimental sites across the Internet.
- Request data archive CD's containing quality assured (QA) experimental data from participating sites.
- Observe graphical summaries of data in the QuickLooks section.
- Examine QA reports that summarize experimental performance and aid diagnostic treatments.
- Examine the standardized data reduction pathway and QA protocols proposed.
- Inspect tabulated site specific performance data with cross comparison by ring and season.
- Examine the QA steps to ensure data quality, reliable operation of the sites and world leading science.
- Download and execute customized database utilities and report generators for automated data analysis.
- Read about the Fair Use policy adopted at BNL for the use and distribution of data derived from the group wide effort that makes up the FACE community.

Robert Cushman, Director of the Carbon Dioxide Information and Analysis Center (CDIAC) at ORNL met with the ECO group at BNL to develop a plan for the archiving of ECO data at CDIAC, as a final data repository.

We are evaluating the use of a general model, WIMOVAC (Windows Intuitive Model Of Vegetation response to Atmospheric & Climate change) as a common framework for data integration and carbon cycle modeling activity. This model has been under development by Steve Humphries for several years prior to his arrival at BNL. WIMOVAC is applicable to a wide range of vegetation and soil types as an experimental tool. The web site now includes documentation describing model assumptions and structures as well has how to operate the software. The concept of a general framework will allow us quickly and easily to compare the performance of different types of models from a variety of experiments.

SPECIFIC ACCOMPLISHMENTS:

- Clear statement of science issues and hypotheses developed by meeting of experts.
- ECO web site on line.
- FACE web site on line.
- WIMOVAC model on line.
- New software systems integrated with field instruments and on line.
- Data QuickLooks graphical summary created and on line.
- ECO site quality assurance performance report defined, created, implemented and now online.
- Software tools for the transmission of experimental data live across the Internet were created and have been transmitting data from Germany (Braunschweig) since September 1999.

LDRD FUNDING:

FY 1999	$346,926
FY 2000	$240,000

Parallel Algorithms for Accelerator Design

J. Glimm 99-10A
R. Samulyak

PROJECT DESCRIPTION:

The purpose of this work is to develop novel algorithms and simulation techniques which can contribute to our knowledge of particle beam interactions in accelerators and the interaction of those beams with targets. These techniques could lead to important scientific knowledge about the Spallation Neutron Source and the proposed Muon Collider. Follow on funding from High Energy Physics in the Office of Science to participate in the interlab development of accelerator codes is likely.

APPROACH:

Particle accelerators have been at the forefront of advances in physics for most of the last century. Efforts to build the next generation of accelerators will involve unprecedented design challenges which can only be met by increased simulation and particle tracking. These problems represent a non-trivial challenge in that space charge and other multiparticle effects must be included for a satisfactory description of the physics. The same applies to the targets themselves for which the particle beams, as deposited, generate large amounts of heating and intense thermal shocks.

ACCOMPLISHMENTS:

Preliminary three-dimensional mercury jet instability calculations in the absence of a stabilizing magnetic field have found parametric regions of stability and instability. The FronTier code developed at Stony book has been ported to The Center for Data Intensive Computing's Linux cluster. Preliminary work on parallel coding algorithms for accelerators has been completed.

PAPERS/JOURNALS/PUBLICATIONS:

B. Cheng, J. Glimm, X.L. Li, and D.H. Sharp, *Subgrid models and DNS studies of fluid mixing*, in Proceedings of the 7th International Conference on the Physics of Compressible Turbulent Mixing, (1999), 2000, submitted.

B. Cheng, J. Glimm, D. Saltz, and D.H. Sharp, *Boundary conditions for a two pressure two phase flow model*, Physica D, (1999), in press.

J. Glimm, J. Grove, X.L. Li, and D.C. Tan, *Robust computational algorithms for dynamic interface tracking in three dimensions*, SIAM J. Sci. Comp., (1999), in press.

J. Glimm, J. Grove, X.L. Li, and N. Zhao, *Simple front tracking*, in Contemporary Mathematics, G.-Q. Chen and E. DiBebedetto, eds., vol. 238, Amer. Math. Soc., Providence, RI, 1999.

J. Glimm, D. Saltz, and D.H. Sharp, *Two-phase modeling of a fluid mixing layer*, J. Fluid Mech., 378 (1999), pp. 119-143.

J. Glimm and D.H. Sharp, *Stochastic methods for the prediction of complete multiscale phenomena*, Quarterly J. Appl. Math., 56 (1998), pp. 741-765.

J. Glimm and D.H. Sharp, *Prediction and quantification of uncertainty*, Physica D, (1999), in press.

J. Glimm, S.R. Simanca, D.C. Tan, F.M. Tangerman, and G. VanDerWoude, *Front tracking simulations of ion deposition and resputtering*, SIAM J. Sci. Comp., 20 (1999), pp. 1905-1920.

J. Walter, J. Glimm, J. Grove, H.-C. Hwang, X. Lin, B.J. Plohr, D.H. Sharp, and D. Yu, *Eulerian front tracking for solid dynamics*, Tech. Rep. LA-UR-99-1796, Los Alamos National Laboratory, Los Alamos, NM, 1999.

LDRD FUNDING:

FY 1999	$125,000
FY 2000 (estimate)	$170,000

Photonic Band Gaps In Nanostructured Materials

J. Davenport *99-10B*
J. Glimm
Y. Deng, SUNY/Stony Brook

PROJECT DESCRIPTION:

Nanostructured materials offer great promise for the control of light (photons) in next generation optical devices. However, the propagation of photons in these structures is not completely understood at present. While studies of transverse electric (TE) modes have been successful there are no comparable studies of transverse magnetic (TM) modes. In cooperation with J. Haus at University of Ohio, Dayton, and Charles Bowden of Redstone Arsenal, we will validate our code through a study of reflection, transmission and pulse propagation through photonic crystals. Effects such as group velocity, pulse dispersion and diffraction will be studied, as will surface modes (relevant to antenna applications), wave guides and optical diodes (relevant to optical computing). In addition, the codes developed under this project will be ported to the 12,000 processor special purpose machine in the RIKEN/BNL Research Center, originally designed for lattice quantum chromo-dynamics.

APPROACH:

The equations to be solved are Maxwell's equations, in the absence of charges, currents, or magnetic poles. The geometric complexity is introduced through the occurrence of discontinuities in the dielectric constant. Typically the interfaces on which the discontinuities occur will be separated by a fraction of a wavelength. In order to extend the theory of these structures into the TM domain we have developed a parallelized, scalable Finite Difference Time Domain (FDTD) code to study photonic crystals. This code is capable of handling complex geometry, realistic initial and boundary conditions, finite size effects, dispersive and nonlinear media, and surface waves.

It is important to use adaptive gridding which conforms to the crystal geometry, including the surface of discontinuity of the dielectric. A regular grid will cover most of the computational domain, while geometric structures will be resolved adaptively using irregular grid elements. We propose to explore the use of a finite volume algorithm, which reduces to a standard finite difference algorithm for the regular grid elements.

ACCOMPLISHMENTS:

Codes for the solution of Maxwell's equations using a parallel algorithm have been designed and partly tested.

PAPERS/JOURNALS/PUBLICATIONS:

Y. Deng, J. Glimm, Y. Wang, M. Eisenberg, A. Grollman, and A. Korobka, *Prediction of protein binding to DNA in the presence of water-mediated hydrogen bonds*, J. Molecular Modeling, **5**, 125-133 (1999).

LDRD FUNDING:

FY 1999	$ 95,000
FY 2000 (estimate)	$140,000

Parallel Algorithms For Biomedical Imaging

J. Davenport *99-10C*
W. B Lindquist
K. Mueller
Wei Zhu (SUNY/Stony Brook)
A. Peskin
M. Mcguigan

PROJECT DESCRIPTION:

The purpose of this project is to develop new improved algorithms for the imaging and treatment of brain disease and functioning. Boron neutron capture therapy (BNCT) is currently under investigation for the treatment of certain brain tumors. The protocol requires both an accurate image of the tumor and the development of a radiation dose schedule customized to individual patients. Both aspects of this problem will be treated by utilizing a fast parallel algorithm along with a simulated annealing procedure to reduce significantly the time required to prepare an individual patient and to provide a three-dimensional image of the tumor suitable for use by physicians. In addition, the software and methodology developed for this project will be utilized to provide new approaches to the automated analysis of data from a series of experiments aimed at studying the effects of radiation exposure on neuronal regeneration. Without new algorithms these data cannot be analyzed effectively.

APPROACH:

Previous analyses have utilized workstations and relatively slow algorithms which have required hours of computer time to complete the task. The approach used here is to parallelize the codes so that modern clusters of workstations can complete the required calculations in approximately one half hour or less. In addition, the possibility of using a simulated annealing algorithm to optimize the dosage will be investigated. This is relatively more risky since algorithms of this type have not been used previously in planning neutron dose.

ACCOMPLISHMENTS:

The codes for running on parallel machines have been developed and partly tested. The latest installed version of treatment planning codes for the Boron Neutron Capture Therapy program represents a factor of five increase in processing speed. Recent work in analysis of rock pore tomographic data based on a medial axis algorithm has focused on characterization of rock pore micro-structures, including coordination numbers and pore and throat size distributions.

PAPERS/JOURNALS/PUBLICATIONS:

A. M. Peskin, and A. B. Andrews, *A Stereographic Visualization Environment and its Applications*, Proceedings of the 1999 Advanced Simulation Technologies Conference, Society for Computer Simulation, San Diego, April 1999

LDRD FUNDING:

FY 1999	$125,000
FY 2000 (estimate)	$180,000

Electron Diffraction Studies of Charge Ordering in Transition-Metal Oxides

Yimei Zhu *99-26*
A. R. Moodenbaugh
J. M. Tranquada

PROJECT DESCRIPTION:

This project combines the analytical power of the new transmission electron microscope (TEM) and sample preparation expertise in the EST Dept., along with x-ray and neutron scattering studies of charge ordering in perovskite-related oxides in the Physics Dept.[1]. Charge ordering, especially in manganese perovskites with colossal magnetoresistance (CMR) and in high temperature superconductors is a subject of widespread interest. The goal is to directly observe charge ordering, including stripe phases, using convergent beam electron diffraction CBED and high resolution imaging methods, both developed recently at BNL [2].

APPROACH:

The project demonstrates the capabilities of the state-of-the-art TEM. An initial study, the charge ordering of Mn cations in $La_{0.33}Ca_{0.67}MnO_3$, is targeted to resolve a controversy over charge ordering models, a Wigner-crystal model based on x-ray diffraction results [3] against a bi-stripe model advocated by electron microscopists [4].

The discrepancies between the two models are striking. Uneven spacing of lattice images in TEM suggests a stripe order for Mn^3, Mn^{4+} [4]. Yet published x-ray diffraction results lead to a Wigner crystal model that is clearly incompatible with the stripe order model [3]. In order to advance the state of the art of x-ray diffraction and TEM techniques, we must identify the source of the discrepancies between models.

Since $La_{0.33}Ca_{0.67}MnO_3$ has a high density of defects, the advantage of TEM is to retrieve single-crystal-like structural information from small areas far away from defects, rather than acquire volume-averaged structural information as obtained by x-ray diffraction. Our approach utilizes unique quantitative TEM techniques, aided by state-of-the-art computer simulation of electron diffraction and high-resolution images on a nanometer scale. To quantify experimental observations, an energy filter and CCD camera are also used.

TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

Parallel beam electron diffraction was used to determine crystal symmetry of the charge-ordered phase, the specimens being temperature T controlled (85K<T<1300K). A systematic study showed that the charge-ordered crystal symmetry is consistent with the Wigner-crystal model [3]. The modulation wave vector was determined to be $\boldsymbol{q} = (0.284, 0, \xi)$ with $\xi = -0.010$. Symmetry-breaking associated with the small component ξ along the c-axis has not been previously observed by high-resolution x-ray or neutron powder diffraction.

To verify the longitudinal displacement inherent in the bi-stripe model, we undertook quantitative analysis of large-angle convergent beam electron diffraction (CBED) at 85K (Fig. 1(a)). Off-zone-axis systematic conditions were used to minimize multiple scattering and to collect diffraction

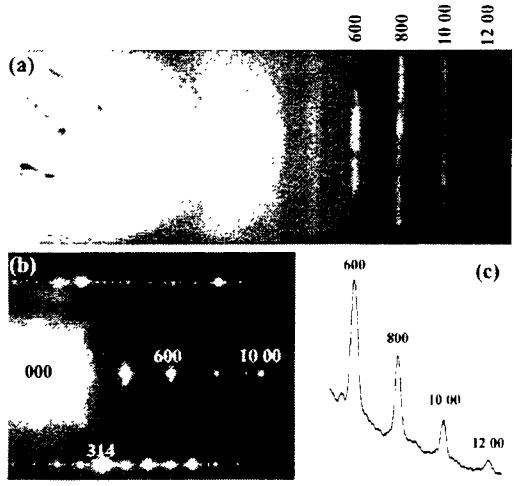


Figure 1. (a) Off-zone axis large angle CBED pattern using zero energy-loss electrons at 85K, showing Bragg reflections as indexed. (b) SAD from the same area showing superlattice reflections due to the charge ordering along the systematic reflection row (l=±1). (c) Intensity profile quantifies the intensities for reflections *of (600) - (1200).* The super-reflections are very weak in the CBED pattern. However, the sharp super-reflection spots acquired from the same area along the systematic rows of *l=±1* in the selected area diffraction (SAD) pattern (Fig. 1(b)) confirmed that the area under investigation was indeed in the charge-ordered state. Quantitative analysis combined with calculations for both SAD and CBED suggest that the intensity distribution in Fig.1(c) is not compatible with the proposed longitudinal displacement and, hence, does not agree with the bi-stripe model.

The key TEM evidence upon which the longitudinal bi-stripe model is based is the difference of spacings between the stripe-pairs of Mn^{3+}-Mn^{3+} and Mn^{3+}-Mn^{4+} along the a-axis measured in TEM lattice images [4]. However, image simulation based on dynamic diffraction theory, incorporating charge and ionicity of atoms, shows that the spacing of stripe-like patterns in a lattice image changes with imaging condition, and does not directly represent atomic positions. This study shows that, without image simulation, observed atomic images and spacings cannot be used reliably to retrieve the atomic coordinates of a complex material.

ACCOMPLISHMENTS:

A DOE 2% New Initiative proposal was presented to DOE, Division of Materials Sciences, as a sole entry from BNL. There were two invited talks, one presented at the Annual Meeting of the Microscopy Society of America, Portland, 8/99, the other to be given at the Materials Research Society Meeting, Boston, 11/99. Paper published: R. Wang, J. Gui, Y. Zhu, and A. R. Moodenbaugh, J. Wuhan Univ., in press. Refereed: R. Wang, J. Gui, Y. Zhu, and A. R. Moodenbaugh, Phys. Rev. B **61** (2000) 11946.

REFERENCES:

[1] See, for example: J. M. Tranquada, et al., Nature (London) **375** (1995) 561.
[2] Yimei Zhu and J. Tafto, Phys. Rev. Lett. **76** (1996) 446.
[3] P. G. Radaelli, et al., Phys. Rev. B **59** (1999) 14440.
[4] S. Mori, et al. Nature **392**, (1998) 473. S. Mori, et al., Phys. Rev. Lett. **81**, (1998) 3972.

LDRD FUNDING:

FY 1999	$86,793
FY 2000 (estimate)	$70,000

Evaluation of a Millimeter Quasi-Optical Source for Non-Destructive Detection & Analysis

M. Ruckman *99-28*

PROJECT DESCRIPTION:

This LDRD program will evaluate the use of a millimeter quasi-optical source for non-destructive materials analysis. Russian Back Wave Oscillator (BWO) technology obtained through the Initiatives for Proliferation Prevention (IPP) program will be used to detect unknown liquid or solid materials in packages. The proposed work will provide data concerning the use of BWO technology for non-intrusive inspection and improve the chances of securing support for future research and development in several areas of interest to the Department of Defense, Department of Energy, and several independent agencies.

Approach: The goal is to acquire the capability to conduct proof-of-principle experimentation with BWO sources small enough to be used in commercial scanning systems. The initial experiments will get optical data for a few selected solids and liquids and the materials used in shipping packages. Materials such as wood, cardboard, leather and paper are chemically inhomogeneous, complex structurally and "rough" when compared to samples normally studied by spectroscopists. Experimentation is necessary to determine how such complexity changes sub-millimeter transmission, beam coherence, or beam polarization. Additional experiments will test the ability of the spectrometer to detect solvents in plastic or glass bottles. Such work would provide data to determine whether a credible case can be made for the further development of a portable BWO-based technology for scanning. The physical data will be used to simulate the performance of a sub-millimeter wave system. LDRD support will also be used to build a small XY stepper to obtain a low resolution image of a test piece to serve as a proof-of-principle imaging system that might be developed as part of a follow-on project.

TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

During FY 1999, efforts focused on (1) receiving, installing, and calibrating the Russian-built spectrometer; and (2) conducting the first measurements on materials of interest to the program. The "Epsilon" spectrometer hardware was received in January 1999, and it was installed in Bldg. 703. Sub-millimeter waves can be considered as ultra far-infrared or micro-wave radiation. The BWO source is sufficiently powerful that it exceeds BNL safety standards, especially when transmitting below 300 GHz. An aluminum enclosure was constructed to shield the experimenter from potentially harmful ultra-high frequency microwaves. The BWO source resembles a traveling wave tube. An electron beam (I = 20-30 mA, E = 2000 V) is directed through a slow wave structure that modulates the electron beam and establishes a periodic EM field. Fluctuations in the beam are amplified at a resonant frequency determined by the geometry of the slow wave structure, energy of the electron beam and strength of the magnetic field in which the BWO electron tube is placed. The BWO is engineered to produce a tunable sub-millimeter wave beam when the electron energy is ramped between several hundred to several thousand volts.

The current set-up measures the optical transmission. If light and dark fringes (oscillations) are observed in the spectrum, physical parameters like the real and imaginary components of the dielectric constant ε' and ε'' (or n and k) can be computed from a fit of the fringes. The sub-millimeter wave signals are detected using a Golay cell. It has a dynamic range of 100,000 and can detect microwatt signals. Detection sensitivity was increased using phase-locked detection. The continuous wave signal of the BWO was chopped. A Ni thin film attenuator is used to prevent the overloading of the Golay cell.

The principal investigator was assisted by Dr. Sergey Lebedev of GPI-RAS (General Physics Institute of the Russian Academy of Sciences, (Moscow, Russia) who visited Brookhaven in June 1999 to help calibrate the "Epsilon" spectrometer and instruct Dr. Ruckman in its use. Dr. Lebedev is one of the specialists at GPI in the operation of this type of apparatus and wrote the GPI-RAS supplied software which performs data acquisition, data storage, and off-line analysis.

Optical extinction data for several materials of relevance to this research has been obtained. Some materials (i.e. cardboard, foam and glass) were chosen because they are used in packaging and the samples ranged in thickness from a millimeter (glass) to a centimeter (packing foam). The rubber and plasticine samples simulate possible threats like explosives. The cardboard, glass, and rubber pieces were sufficiently flat and of uniform thickness to display interference fringes that were used to compute a dielectric constant. Since the absorbance of a composite material (e.g. a sandwich of rubber between two slabs of cardboard) can be deduced by addition of the product of the absorption coefficient and thickness of each component, the research indicates that a sandwich of card-board, packing foam and rubber can be distinguished from a sandwich containing no rubber or plasticine.

Future LDRD work in FY 2000 will build on basic spectroscopic measurements like those shown above. The investigator is seeking samples to determine if such microwave beams can detect the deterioration of insulating materials in electrical cabling. If this exploratory work is successful, it could lead to the development of new equipment and techniques to detect faults in wiring and cable harnesses used in many facilities (i.e. nuclear power plants) and vehicles (i.e. aircraft).

ACCOMPLISHMENTS:

A proposal entitled "Quasi-optical Microwave Imaging for Concealed Threat Agent Detection" was submitted to the Department of Energy, Office of Nuclear Non-Proliferation (NN-20) for consideration as a FY 2000 New Start.

LDRD FUNDING:

FY 1999	$ 84,768
FY 2000 (estimate)	$ 60,000

Microdistribution Studies of ^{10}B for Boron Neutron Capture Therapy Using Transmission Electron Microscopy

Ruimei Ma *99-40*
Yimei Zhu
Joseph S. Wall
James F. Hainfeld

PROJECT DESCRIPTION:

In radiotherapy the dose that can be delivered to tumor cells is limited by the tolerance of the normal tissues within the radiation field. Boron neutron capture therapy (BNCT) is based on the neutron capture reaction ^{10}B $(n,\alpha)^7Li$. The combination of high LET and a short range of the alpha (α) and ^7Li particles increases the statistical chances that ^{10}B-laden tumor cells will be rendered non-clonogenic ("killed") while contiguous, ^{10}B-poor tissues will be spared. The microdistribution of ^{10}B in both tumor and normal tissues is of critical importance to BNCT. The objective of this LDRD is to conduct a feasibility study on the ppm intracellular boron detection using two high-performance electron microscopes at BNL.

TECHNICAL PROGRESS AND RESULTS – Fiscal Year 1999:

Purpose: to measure the ^{10}B concentration in single cells and contiguous zones of extracellular matrix using the TEM in the Department of Applied Science and the STEM3 in the Biology department.

Approach: 1) obtain boron detection limits and the radiation sensitivity of boron compounds of interest in tests of non-tissue samples, 2) develop a protocol for tissue specimen preparation, 3) detect boron in tissue samples.

Technical Progress and Results: During FY 99, research was focused on determination of the measurement sensitivity for boron in a carbonaceous specimen. The initial test was conducted on specimens consisting of a very thin layer of boron deposited onto a carbon film, which is supported on a TEM grid. The total specimen thickness of around 50nm should be near optimum for 300kV EELS spectroscopy or mapping of boron.

Fig.1(a) shows an electron energy-loss spectrum acquired from a test sample consisting of a 50nm carbon layer and a 0.1nm boron layer. Only the carbon peak at ~284ev is visible. After background-subtraction of the carbon, we observed a broad boron peak at an on-set of ~188eV, shown in Fig.1(b). Quantitative analysis showed that the atomic ratio of boron and carbon was about 0.2%, as expected from the sample compositional geometry.

Next, we tested a biological sample which had tobacco mosaic virus (TMV) deposited on a thin (2-3nm) carbon film and "stained" with 0.5% BPA. Fig.1(c) shows a bright-field image of the TMV, acquired from a CCD camera at a magnification ~200kx. Fig.1(d) is the boron map acquired with the Gatan Imaging filter from the same area shown in Fig.1(c). The bright band-contrast in Fig.1(d) represents the high concentration of boron in the area. We have not quantified the B concentration for TMV.

In an optimized TEM/EELS setting, we found that a boron concentration of about 0.2% (2000ppm) should be measurable at 10% accuracy, and 1 μm spatial resolution. Since the sensitivity should depend on incident-beam current but not diameter,

similar measurements should be possible with spatial resolution down to 1nm provided radiation damage is not a problem.

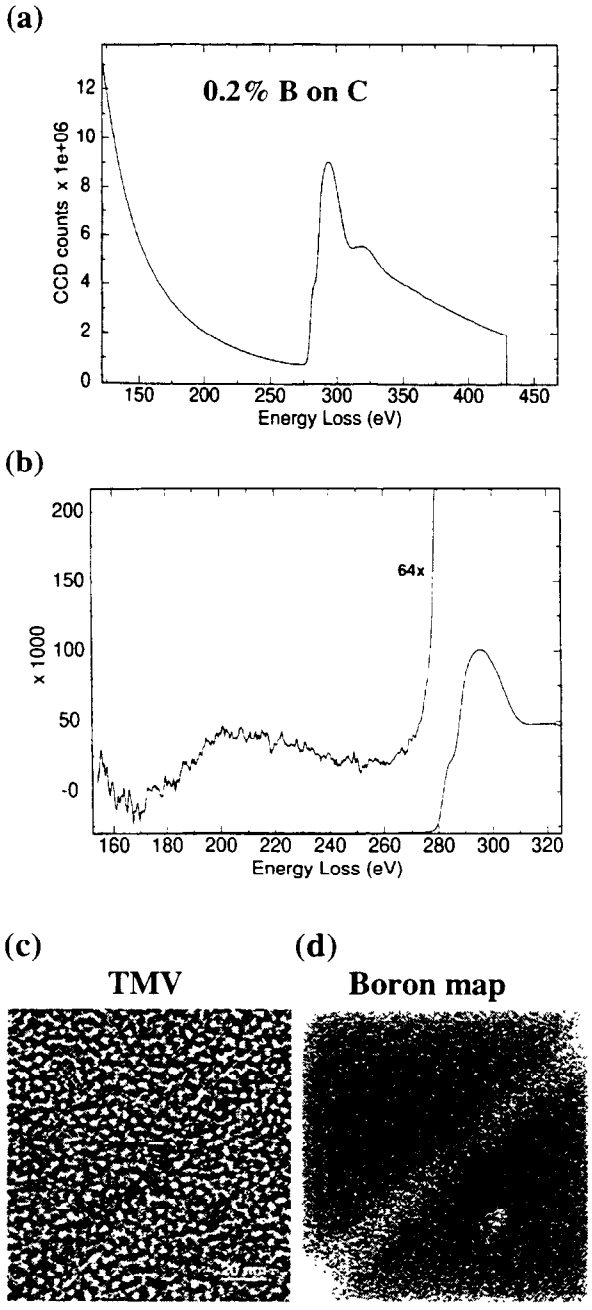


Figure 1 (a). Electron energy-loss spectrum of a test sample containing 0.2% Boron on a carbon film. (b): After background subtraction. Note, the B-edge is on a reduced scale. (c): TEM image of a TMV; (d): boron distribution of the same TMV.

BPA was imaged in STEM1 in Biology to test its radiation sensitivity and found to have no significant mass loss upon irradiation. The metallic boron specimens were also very stable against spallation in the electron beam.

In order to prepare the proper sample for electron microscopic analysis of tissues for boron content, we have arranged to use suitable cryoultramicrotomes at the National Institutes of Health in Bethesda, MD.

Several animals were injected with 10-BPA, N-BPA, and ZnTCPH (porphyrin), and samples from liver, cerebrum and spleen collected and rapidly frozen. These have been analyzed by DCP for bulk boron content. These samples will be transported to NIH and ultrathin cryosections prepared and mounted on electron microscope grids for analysis at BNL.

In parallel with the above research activities, an alternative boron mapping strategy was devised after searching the literature and available techniques. A mass spectrometer microscope (MSM) has been invented. A second-generation instrument is now completed that adds the more sensitive channel plate detector. We have consulted with persons in the Chemistry Dept. familiar with mass spectrometer design, and arranged with DAT use of their suitable excimer or pulsed lasers. Future plans for the MSM will include testing its sensitivity, addition of laser ablation if required, calibration, improving collection electronics, and adaptation to a light microscope.

LDRD FUNDING:

FY 1999	$117,614
FY 2000 (estimate)	$ 60,000

Efficacy of Unidirectional Microbeam Radiation Therapy in Treating Malignant Tumors: Preclinical Studies in Rats and Mice

F.A. Dilmanian *99-41*
B. Ren
L. Peña
In collaboration with: T. Bacarian, J. A. Coderre, W. Estrada, S. Martinez, G. M. Morris, I. Orion, S. Packer, P. Recksiek, E. M. Rosen, P. Sathé, J. Tammam, D. White, and Z. Zhong

PROJECT DESCRIPTION:

In conventional radiation therapy, damage to normal tissues surrounding the tumor is thought to stem largely from injury to endothelial cells, leading to disruption of blood perfusion end eventually necrosis. Microbeam Radiation Therapy (MRT) seems to allow endothelial cells in the normal tissue to regenerate from surviving cells between the beams and thereby sparing the micro-vasculature and ultimately normal tissues. MRT uses arrays of parallel, microscopically thin slices of synchrotron x rays. Microbeam arrays used at the National Synchrotron Light Source (NSLS) are typically 30-100 μm wide and up to several centimeters high, spaced at 100-300 μm intervals center-to-center, with a median beam energy of 65-130 keV. Unidirectional microbeam (MB) irradiation of animals at the NSLS showed two remarkable effects: a) exceptional sparing of normal tissues, and b) tumor ablation or palliation in rats with intracranial or subcutaneous 9L gliosarcoma (9LGS) tumors, while retaining the tissue-sparing effects to the surrounding normal tissue.

APPROACH:

The goals of the present LDRD have been: a) to establish more quantitatively the validity of the two effects of MRT, namely sparing normal tissues and killing tumors in the central nervous system (CNS) by irradiation from a single direction; b) to establish the biological bases of the two effects of MRT, and c) to establish the generality of the tumorocidal effect of unidirectional MRT in several tumors other than 9LGS.

PROGRESS:

a. Technical

A multi-slit collimator was developed for the program by Tecomet Thermo Electron. Because of the exposure time saved, we now use more beam filtration, cut back on the dose rate, and increase the beam's median energy (from 65 keV to 120 keV). This increases the depth of the dose penetration from about 3 cm half-value tissue layer to about 5 cm. Progress was also made in our Monte Carlo simulations, thanks to the works of I. Orion, B. Ren, and T. Bacarian. We now calculate dose in subjects of relatively complex shapes.

b. Studies with normal tissues

i. Radiation tolerance of rat and gerbil spinal cord: The gerbil experiment showed a 3-fold advantage for microbeams versus broad beams using the same total absorbed energy; we used a broad beam of 4-mm width, and a microbeam array of 11-mm frame width. This means a seven-fold advantage for microbeams when compared for the same frame widths. The rat experiments also show significant advantage for microbeams.

ii. Radiation tolerance of the normal rabbit eye
In this work, a collaboration with Dr. S. Packer of North Shore Univ. Hospital, rabbit eyes were irradiated with microbeams or broad beams. The results show no damage to the retina at 625 Gy microbeams a year after irradiations; the corresponding damage to the retina from 312-Gy broad-beam irradiation

was substantial. The histology work is being done in collaboration with Dr. Daniel Albert of Univ. of Wisconsin.

iii. Threshold for necrosis in the rat brain: Rats were irradiated with crossfired microbeam pattern at the cerebrum to measure the threshold be brain tissue necrosis, and with unidirectional microbeams in their cerebellum in a pattern in which the dose varied from one microbeam to the adjacent one to measure the threshold for direct neuronal cell death. Neuronal cells were counted on each slide with the help of Steve Martinez from Stony Brook. Manuscript is in preparation.

iv. Proliferation of the endothelial cells

We used BrdU to label the proliferating cells, and lectin to label endothelial cells. The goal was to find the temporal and the spatial pattern of endothelial cell proliferation, to correlate the spatial pattern with that of MB geometry, and to verify that the proliferating cells are endothelial cells. The rats were irradiated in their cerebellum, and were injected intraperitoneally with BrdU in the following time points: 1d, 1.5 d, 2 d, 2.5 d, 3 d, 3.5 d, and 4 d. Results are being analyzed.

v. Radiation tolerance of the normal rat skin

The end point was the appearance of moist desquamation on the skin. The results indicate that the ED50 dose for moist desquamation is about 850 Gy for microbeams and 40 Gy for broad beams from the NSLS. This leads to more than 20-fold higher tolerance to microbeams versus broad beams, which, when normalized to the same irradiation volume, gives a 6-fold advantage to microbeams.

c. Studies with animal tumor models:

i. Subcutaneous rat 9L glioblastoma: Rats were irradiated with microbeams and broad beams after being inoculated with 9LGS cells under the skin. Complete tumor control in each experiment was achieved with microbeams at 150 Gy (27-μm beam, 100-μm spacing), and 250 Gy (90-μm beam, 300-μm spacing). Broad beams at the RT-100 machine (low energy) controlled the tumor at 20 Gy.

ii. Intracranial rat CNS-1: The cure rate has been about 45% with microbeams of 100 and 150 Gy. The work was hampered by problems with tumor inoculation, that we hope to solve.

ACCOMPLISHMENTS:

The therapeutic index (i.e., the maximum dose tolerated by normal tissue, divided by the minimum dose that controls the tumor) is 6.0 for microbeams, compared to 1.6 for broad beams. Our results enhance our understanding of the microbeam effects, direct us in the path of new findings, and serve as material for several publications. A grant proposal was submitted to the Army's Breast Cancer Research Program in June 2000, and one is being prepared for the OBER, U.S. DOE. Three manuscripts are in preparation.

PAPERS/JOURNALS/PUBLICATIONS:

A.B. Rosenfeld, G. I. Kaplan, T. Kron, B.J. Allen, F. A. Dilmanian., I. Orion, B. Ren, and A. Holmes-Siedle. "MOSFET Dosimetry of an X-ray Microbeams" , IEEE Trans. Nucl. Sci., NS-46, N6, 1774-1780, 1999.

F.A. Dilmanian, G.M. Morris, G. LeDuc, X. Huang, B. Ren, T. Bacarian, J.C. Allen, J. Kalef-Ezra, I. Orion, E.M. Rosen, T. Sandhu, H.L. Shivaprasad, X.Y. Wu, and Z. Zhong. Response of avian embryonic brain to spatially segmented x-ray microbeams. Cellular and Molecular Biology (accepted).

I. Orion, F.A. Dilmanian, A. Rosenfeld, F. Telang, B. Ren, and Y. Namito. Monte Carlo simulation of dose distributions from a synchrotron-produced micro-planar beam array using the EGS4 code system. Phys. Med. Biol. (accepted).

LDRD FUNDING:

FY 1999	$119,571
FY 2000	$130,000

Toxin Bio-Information Resource

S. Swaminathan *99-45*
Enrique Abola

PROJECT DESCRIPTION:

The goal of this work is to establish an informational resource primarily focused on molecular information about toxins and other virulent factors that are the natural products of potential biological warfare agents. The major objective of this LDRD is to develop a robust bio-informational resource that will collect, assimilate, synthesize, analyze and disseminate the basic molecular and structural information about potential biological warfare (BW) agents.

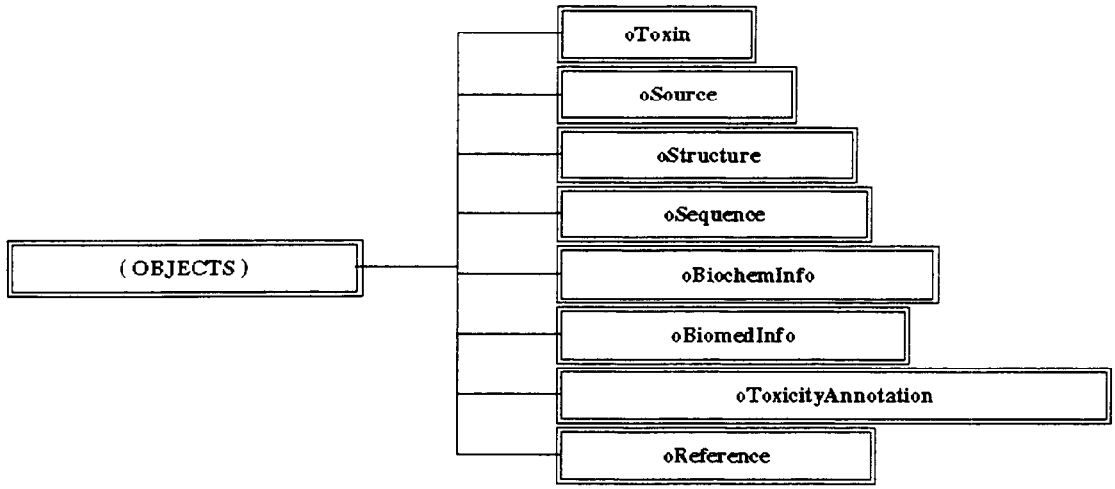
TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

Purpose: Recent events have shown that bio-warfare threat extends beyond the use of virulent bacterial strains that are used in wartime. Recent advances in recombinant DNA technology have opened up numerous possibilities for production of bioengineered pathogens or their products on large scale. Chimeric molecules form another form of threat wherein the virulent domain of a toxin is hidden in what is otherwise a non-pathogenic protein. The aim of this project is to integrate all relevant cellular, molecular and structural information about toxins and related proteins into one centralized database that could be used as an expert knowledge based system to learn about potential warfare agents.

Approach: The goal will be achieved by establishing a database in several stages. The first step is to design and implement a highly curated Object-Oriented Database System (OODB) which involves developing a schema consisting of different objects. Then a system will be devised for identifying and maintaining important links between database objects and other information resources. Using the OODB and protein modeling work, data will be generated on the feasibility of engineering chimeric molecules that could be used as new and powerful BW agents by enemy states. Such analysis will be used to identify potential biological warfare agents. Information and data will be available in the database to identify and understand common motifs and structural patterns in these agents which would lead to developing counter measures such as detectors, drugs and vaccines.

Technical Progress and Results: During the fiscal year 1999, we began by collecting information on a few select toxins. We have analyzed these data in order to develop a schema for the object oriented database. Based on the information and our analysis, we have developed a schema of the database which is being constantly revised and improved to make the database all encompassing and efficient. A pictorial representation of the basic level of this schema is given below. Each box on the right is an object itself and has various attributes and links. In addition to the information from other databases, we have included our own annotations, which are derived from our literature search.

Object Generalization Hierarchy



Each of the objects on the right has information stored in various attributes which have links to external databases. For example, the sequence and structure objects have links to similar structures and sequences. Most of these have been gathered by us. Our future aim is to give pictorial representation of structure motifs included as separate objects.

We are now concentrating our efforts on collecting data on bacterial toxins which are toxic to humans. We will expand this to other organisms and also to toxins that are toxic to animals.

FOLLOW-ON FUNDING:

A proposal has been submitted to DARPA on the "Design and Implementation of Toxin Knowledge Base" in collaboration with SUNYSB which is still under review.

LDRD FUNDING:

FY 1999	$74,855
FY 2000 (estimate)	$75,000

Experimental and Theoretical Investigations of Transition Metal Oxides

J. P. Hill and *99-46*
D. Gibbs

PROJECT DESCRIPTION:

Statement of Work: The goal of this project is to push forward the development of new resonant x-ray scattering techniques in the study of transition metal oxides.

Approach: Systematic studies of the $Pr_{1-x}Ca_xMnO_3$ system were planned to investigate the relative importance of charge and orbital order. The theoretical development of the resonant scattering technique was to be pursued simultaneously.

TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

i) Doped Manganites
Studies of $Pr_{1-x}Ca_xMnO_3$ with x=0.25, 0.3, 0.4 and 0.5 were performed. The results for the x=0.4 and 0.5 have been accepted for publication in Physical Review Letters [1].

In the x=0.4 sample, the semiconductor-to-insulator transition at T_O=245 K was investigated. Below T_O, the charge and orbital intensities follow the same temperature dependence, though long-range orbital order is never achieved. Above T_O, the charge order fluctuations are more highly correlated than the orbital fluctuations (Figure 1), suggesting that the charge order drives the orbital ordering.

ii) Theoretical Progress
Since our initial work, a debate has emerged in the literature as to the origin of the resonant enhancement of the scattering

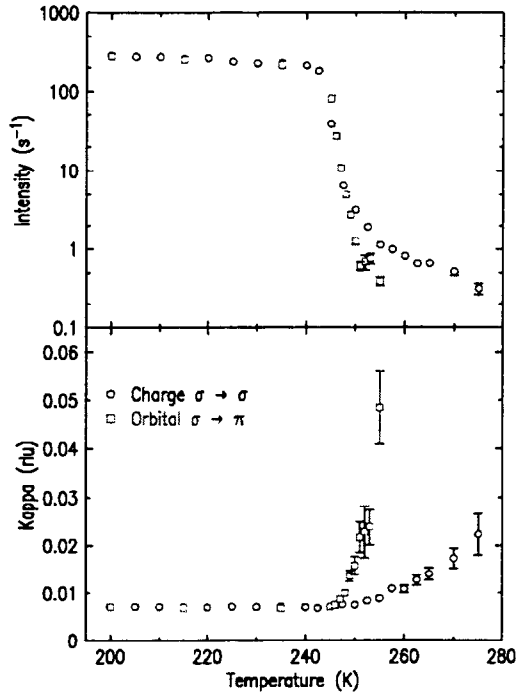


Figure 1. Temperature dependence of the peak intensities (top) and half-widths at half maximum (bottom) of the charge (blue) and orbital (red) for $Pr_{0.6}Ca_{0.4}MnO_3$.

signal. It is our belief that the precise mechanism is not relevant for understanding the physics of the materials. Nevertheless, this is an interesting question. One method for resolving the debate is to compare predictions for the resonance lineshape with experimental data. To this end we have made available high-energy resolution (0.2 eV) data to both theoretical groups.

Also LDRD funds were used to host Sumio Ishihara at BNL for 5 weeks. Ishihara (U. Tohoku, Japan) is the leading theorist in the study of resonant scattering as applied to charge and orbital order.

iii) Titanates
Preliminary work has begun on two titanates, $LaTiO_3$ and $YTiO_3$. Orbital order was observed in the YTiO3 system but not

in the LaTiO3 system. These results shed light on the very different ground states of these isomorphic systems.

iv) APS Beamline
The x-ray group is partners in a new beamline at the Advanced Photon Source (APS) completed this year. The first experiments showed that the signal rates are 50x higher for these types of experiments than at the NSLS.

ACCOMPLISHMENTS:

Funding: This work formed part of the basis for a proposal to the DOE Complex Materials and Cooperative Phenomena initiative. This was successful. The BNL portion of the award was ~$240k p.a.

Invited Talks: Talks given in the last year on work supported by the LDRD include:

1. CREST Workshop, Kobe, Japan November 1998.
2. Plenary Talk, International Conference on Synchrotron Radiation Studies of Materials Science, Kobe, Japan, November 1998.
3. Seminar, Spring 8, Himeji Japan, November 1998.
4. Exotic Oxides Workshop, BNL, March 1999.
5. APS March meeting, Atlanta, Ga, March, 1999. (contributed).
6. Seminar, Dept. Applied Physics, Cornell Univ., March 1999.
7. Ringberg Workshop on Manganites, Munich, Germany, April 1999.
8. NSLS Users Meeting, BNL, May 1999.
9. Plenary Talk, Rare Earth Research Conference, ANL, July 1999.
10. Gordon Conference on X-ray Physics, Plymouth State College, July 1999.
11. Science and Technology of Magnetic Oxides, La Jolla, Ca., July 1999.
12. International Union of Crystallography, General Congress, Glasgow, Scotland, August 1999.
13. X99, International Conference on X-ray and Inner Shell processes, Chicago, Il, August 1999.
14. International Conference on Solid State Spectroscopy, Stuttgart, Germany, September 1999.

Publications

1. M. v Zimmermann, J.P. Hill, D. Gibbs, M. Blume *et al.* Phys. Rev. Lett (accepted).
2. J.P. Hill *et al.*, Phys. Rev. B. (accepted).
3. J.P. Hill, to be published in Conference Proceedings of X99, Elsevier Press.
4. J.P. Hill *et al.* Jpn. J. Appl. Phys. **38** 118 (1999).
5. Y. Murakami, J.P. Hill, D. Gibbs, M. Blume *et al.*, Jpn. J. Appl. Phys. **38** 360 (1999).
6. D. Gibbs, J.P. Hill, C. Vettier, chapter in "Hard X-ray Scattering at Third Generation Sources", John Wiley (in press).
7. D. Gibbs, J.P. Hill, C. Vettier, Phys. Stat. Sol. **215** 667 (1999).
8. H. Nakao, M. v. Zimmermann, J.P. Hill, D. Gibbs *et al.* Phys. Rev. Lett., (to be submitted).

Supported Researchers:
1 Post-doc. (M. v. Zimmermann)
1 Summer visitor (theorist), 5 weeks
1 Summer visitor (experimentalist) 3 weeks.
Travel to Advanced Photon Source for experiments.
Travel to selected meetings.

LDRD FUNDING:

FY 1999	$84,381
FY 2000	$60,000

Pulsed Laser Deposition Facility

Peter D. Johnson 99-48
Barrett O. Wells
T. Venkatesan

PROJECT DESCRIPTION:

Studies of correlated electron systems represent one of the forefront challenges in Condensed Matter physics at the present time. In particular, studies of the high T_c superconductors are the subject of a huge research activity. Photoemission represents one of the primary tools available for the study of these materials. However, one of the limitations of photoemission is that it requires well-defined surfaces. To date therefore, the great majority of photo-emission studies have concentrated on the cuprate $Bi_2Sr_2CaCu_2O_{8+\delta}$, which is cleavable. On the other hand, few of the high T_c neutron scattering studies have been carried out on this material because of the difficulty of getting large samples. Indeed neutron scattering has tended to concentrate on $La_{2-x}Sr_xCuO_4$. Unfortunately, the latter materials do not cleave so easily. It is thus important to bridge the gap between the two probes because much of the pioneering work at BNL on Stripes was carried out on the $La_{2-x}Sr_xCuO_4$ and related materials. It is, therefore, intended that growth of the $La_{2-x}Sr_xCuO_4$ type materials will be one of the primary objectives of the Pulsed Laser Deposition (PLD) work.

TECHNICAL PROGRESS AND RESULTS - Fiscal Year 1999:

Purpose: The project, which represents a collaboration between the University of Connecticut and the Physics Dept., is to establish an in-house materials growth capability based on the PLD. Another collaboration is also being established with the University of Maryland, where much of the U.S. effort in PLD is centered. The ultimate aim is to be able to grow in-situ samples for use in different experiments at the National Synchrotron Light Source. The first objective is to grow samples that can be used in probes that are less sensitive to the surface condition. These techniques include optical conductivity and x-ray scattering. However, a long-term concern is whether or not the texture of the surface will allow photoemission studies.

Approach: The facility is currently being established in the Physics Department. Ideally it would be constructed directly on the UV floor at the NSLS. However, various safety issues make this a more difficult approach during the initial commissioning stage. The plan, therefore, is to commission the facility and grow samples in the Physics Department and then transfer them to various experimental end stations in some form of vacuum suitcase. When sufficient experience has been acquired, we will review the possibility of moving the facility to the NSLS.

Status: A room in the Physics Department has been equipped with all of the appropriate safety equipment and the laser has been installed. In the next few weeks, we anticipate a visit from the Lambda Physik laser engineers to commission the machine. This will allow the production of samples to begin almost immediately.

In the meantime Barry Wells, funded from the LDRD program, has visited the University of Maryland to the rudiments of growing crystals. Several samples of strained $La_{2-x}Sr_xCuO_4$ were prepared by growing on different substrates and these are now being investigated using x-ray

scattering. The strain, the equivalent of applying pressure, has the effect of modifying the transition temperature, T_c, of the material. X-ray scattering studies of strained $SrTiO_3$ have also been completed.

Future Plans: Over the next year it is intended to get experience in growing films under different growth conditions. The properties of the films will be determined using resistivity measurements and X-ray diffraction as a structural probe. When good growth conditions have been established initial measurements will be made at the NSLS using the technique infra-red spectroscopy.

ACCOMPLISHMENTS AND FOLLOW-ON FUNDING:

The work on $SrTiO_3$ is being submitted for publication: - "Extreme strain effects on the structural phase transitions of SrTiO3 thin films," B.O. Wells, M. vonZimmermann, S.M. Shapiro, Y. Zhu, A. Clark, and X.X. Xi.

The Condensed Matter Physics program has been successful in obtaining new money through the recent Complex Materials Initiative. A key component of the proposal was the stated intention of studying new materials fabricated using the technique of Pulsed Laser Deposition.

LDRD FUNDING:

FY 1999	$122,342
FY 2000 (estimate)	$ 60,000

Ultrashort Electron Bunch Length Monitor

William S. Graves 99-50
Louis F. DiMauro
Richard Heese
Erik D. Johnson

PROJECT DESCRIPTION:

The particle beams required for both next generation light sources based on free electron lasers and for future linear colliders will consist of ultra-short, intense electron bunches. There is widespread interest among DOE laboratories in developing instrumentation to accurately measure the properties of these beams. The Deep Ultra-Violet FEL (DUV-FEL) currently nearing completion at the NSLS will produce a beam that is well suited for development of new diagnostics, and an effort is underway to develop new instrumentation for sub-picosecond electron beam measurements.

Simulations indicate that the electron bunch compressor at the DUV-FEL can produce electron bunches as short as 200 fs FWHM. These short bunches have high peak currents of a few kiloamps that are very important for the success of single pass FEL amplifiers. Bunch lengths on this scale cannot be measured by traditional accelerator methods or by the fastest streak cameras. However, optical methods developed by laser scientists to measure ultrashort light pulses are applicable. The idea is to produce a short pulse of radiation from the electron bunch that accurately reproduces its temporal profile. The temporal shape of this light pulse is then measured via optical gating of a synchronized laser in a nonlinear crystal.

APPROACH:

The best existing time-measurement instrument is the streak camera, which can accurately measure bunch lengths longer than about 2 ps. To extend this range to shorter timescales, the first of several approaches under investigation utilizes an ultra-short titanium:sapphire laser pulse that is synchronized with the electron beam to gate a radiation pulse produced by the electrons into a slow detector. The electron pulse shape is mapped by varying the delay of the laser with respect to the electrons. Two key requirements of this experiment are the sub-picosecond time synchronization of the electron beam and laser, and that the radiation produced by the electron beam accurately reproduce the electrons' profile. The required time resolution is achieved by splitting the laser gating pulse from the same laser pulse that creates the electron beam on the photocathode. This provides absolute synchronization. Two methods of producing a suitable radiation pulse from the electron beam will be tested. The first is to use optical transition radiation produced by the electrons transiting a thin foil. The second method is to use synchrotron radiation produced in a short undulator. This method has the advantage of producing more optical power, thus increasing the measured signal, and being nondestructive to the electron beam.

PROGRESS:

The successful completion of the ultra-short bunch length monitor depends upon completion of the accelerator installation, commissioning of the titanium:sapphire laser, construction of laser transport lines to

the end of the linac, reconstruction, measurement, and magnetic shimming of an existing short undulator, design and construction of in-vacuum diagnostics for the undulator, construction of vacuum parts for the transition radiation foil, optical transport elements to bring the electrons' radiation to the experimental area, and purchase of an optical spectrometer and detectors for the gated light.

Ongoing progress in FY99 includes extensive development and commissioning of the titanium:sapphire laser. It is expected to be finished in January, 2000, at which time first beam studies will begin. A 12-period undulator has been extensively rebuilt and is currently having its magnetic field mapped and shimmed to meet the necessary electron trajectory tolerance. It is expected to be ready for installation in Spring, 2000. The in-vacuum diagnostics for the undulator have been designed and are under construction. A large optical table has been installed and preparations are underway to install the components upon it.

ACCOMPLISHMENTS:

In FY99 we have completed installation of the accelerator and it is now undergoing commissioning. The transition radiation monitor has been designed, built, and installed in the linac. Design of the optical transport for both the transition radiation and the undulator radiation is complete and all parts and detectors have been procured. A graduate student from Duke University has recently joined the group and his thesis will be based on these beam measurements. We have refined our understanding of the coherent undulator spectrum emitted and have submitted a paper to Physical Review. This work has recently received external funding from a national FEL collaboration to develop complementary methods of measuring ultra-short electron bunches and synchronizing them with lasers.

PAPERS/JOURNALS/PUBLICATIONS:

"Coherent Off-Axis Undulator Radiation from Short Electron Bunches," C.P. Neuman, W.S. Graves, P.G. O'Shea, submitted to Physical Review Special Topics – Accelerators and Beams

LDRD FUNDING:

FY 1999	$110,200
FY 2000 (estimate)	$ 65,000

High Gain FEL Amplifier

George Rakowsky *99-51A*
William S. Graves
Erik D. Johnson

PROJECT DESCRIPTION:

For High Gain Free Electron Lasers to work as single pass devices at short wavelengths, very long wigglers will be required for the amplifier. These devices would (in principle) be most efficient if they can be built without gaps for diagnostics and trajectory correction magnets. Although the idea has been around for some time, this approach has never been demonstrated experimentally, which is the aim of this project.

APPROACH:

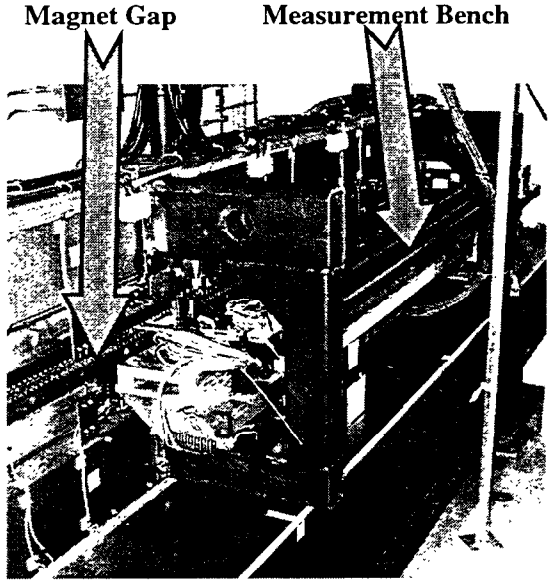
As a starting point, we have obtained the 10 meter long NISUS wiggler (from a canceled Army program) to use for this proof-of-principle experiment. If the device can be measured and shimmed to the tolerances required for an FEL amplifier it would demonstrate the viability of the long seamless wiggler design approach. Our measured data will be used as input to model an FEL amplifier, which will help establish realistic expectations for FEL performance.

PROGRESS:

Magnetic measurements have been undertaken in collaboration with STI Optronics. Because the device is so long, a 3-meter long scanning hall probe is shifted along the undulator in four overlapping steps. Part of the difficulty of these measurements is assuring that the alignment of the bench is properly referenced each time it is moved to a new measurement location. There is some overlap from one measuring position to the next to provide a complete magnetic map of the device. NISUS was built in 16 segments, each with its own four-wire steering section built into the vacuum chamber. After initial measurement, magnetic shimming will be performed with the goal of achieving a trajectory walk-off of less than 30 μm per steering section.

ACCOMPLISHMENTS:

To facilitate this measurement, wide gap stanchions were prepared and installed on NISUS so the measurement bench can be placed inside the stanchions to allow a continuous scan with the existing equipment. The set-up is shown in the following photograph.



Photograph of the 3-meter long magnetic measuring bench on the NISUS table.

The measurement system has been installed and an initial field map obtained. In its "as measured" state, trajectory errors of more than 10 mm (10,000 μm!) for 140 MeV beam energy were obtained with optical phase errors the order of hundreds of degrees. This

would be unacceptable for use as an FEL. Analysis of the data is underway to determine the proper shimming to bring these parameters into specification.

PAPERS/JOURNALS/PUBLICATIONS:

"Research Opportunities for the BNL DUV-FEL," E.D. Johnson, Presented at FEL 99 Conference, Hamburg Germany, August 23-27 1999.

LDRD FUNDING:

FY 1999	$100,000
FY 2000 (est)	$100,000

Deep Ultra-Violet Free Electron Laser Optimization

Erik D. Johnson *99-51B*
William S. Graves
Brian Sheehy
Li Hua Yu

PROJECT DESCRIPTION:

Free Electron Lasers represent the frontier in accelerator based light sources. While there are many theoretical studies, there are relatively few experiments at short wavelength. None have yet monitored the FEL process as the photon and electron beams propagate though a continuous amplifier. This is especially important if tapering is to be used to provide energy extraction beyond FEL saturation. This work examines these issues experimentally and will provide data that can be used to qualify models for projecting the performance of future light sources.

APPROACH:

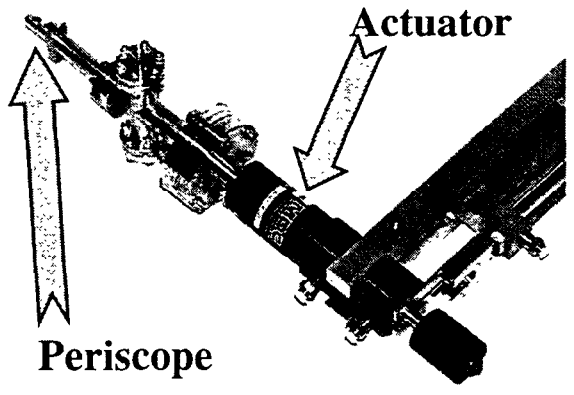
A critical element of the Deep Ultra-Violet Free Electron Laser (DUV-FEL) project is the optical amplifier. This requires a long magnetic undulator, electron beam diagnostics and controls, and an optical system to collect the light from the FEL and preserve its coherence as it is delivered to the experimental station.

As a starting point, the US Army has transferred ownership of the NISUS undulator to BNL. This 10 meter long undulator is very flexible, and can be used to explore the way in which electron beam parameters influence FEL output. The vacuum system and diagnostics will be developed and assembled in the existing undulator. Light from the FEL will be relayed out to an optical table with a simple first surface mirror transport line. Initial experiments will be conducted in the infra-red and visible due to the ready availability and high quality of optical diagnostics.

PROGRESS:

NISUS was built in 16 segments, each with its own four-wire steering section built into the vacuum chamber. Each section also has a port for a diagnostic probe to be inserted to measure the position and profile of the electron beam. We have adapted designs from previous projects including the HGHG experiment and VISA to apply to the DUV-FEL.

The monitors use YAG scintillating screens in a periscope pop-in monitor that has a second mirror position to extract FEL radiation for analysis. To the extent possible, commercial components are used in the design to keep the cost down. The prototype for these monitors is shown in the following figure.

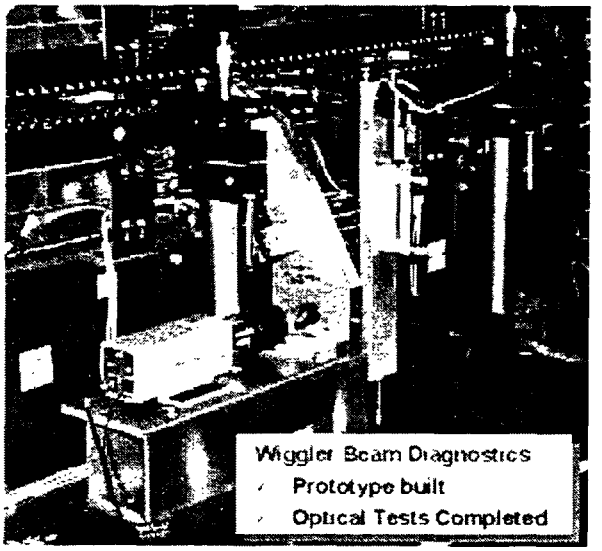


Photograph of the pop-in monitor developed for use in the NISUS undulator.

ACCOMPLISHMENTS:

We have completed modifications to the vacuum system to allow installation of beam monitors throughout the amplifier.

The prototype monitor was installed in a full section chamber prototype to make sure that the vacuum loading from the bellows did not shift the chamber. These tests showed that the current design is sufficiently stable to be replicated for the rest of the undulator.



Photograph of the prototype pop-in monitor installed for testing in a section of NISUS undulator vacuum system.

PAPERS/JOURNALS/PUBLICATIONS:

"Research Opportunities for the BNL DUV-FEL," E.D. Johnson, Presented at FEL 99 Conference, Hamburg Germany, August 23-27 1999.

LDRD FUNDING:

FY 1999	$400,000
FY 2000 (est)	$300,000

Development of High Brightness Electron Sources

Ilan Ben-Zvi *99-53*
Marcus Babzien
Robert Malone
Xijie Wang
Vitaly Yakimenko

PROJECT DESCRIPTION:

Statement of Work: The purpose of this LDRD project is to make a decisive step towards brighter electron beams. The development of diagnostics that image the electron beam density in multi-dimensional phase space (up to 6-D) and use it to perform a 'non-linear emittance correction' will allow us to improve the brightness of electron beam bunches.

TECHNICAL PROGRESS AND RESULTS:

Purpose: The specific purpose of this project is to improve the brightness of laser-photocathode RF electron guns.

Background: The critical element for the next-generation of light-sources and future High-Energy linear-colliders is the generation of high brightness electron beams.

Objectives:

- High–brightness electron beams is the single most important technology required for the implementation of short wavelength FELs.
- A full-sized X-ray FEL User Facility requires further advances in high-brightness electron beams to reduce the required linac size.

- FISCAL YEAR 1998:

In the initial period of the program on non-linear emittance correction, the main emphasis was placed on the improvement of the various components of the accelerator. The goal is to achieve the necessary level of stability and accuracy of the control for tomographic recovery.

- FISCAL YEAR 1999:

1. Beam transport analysis and control.
The data of quadrupole lenses settings and beam size measurements on multiple beam profile monitors over the entire Post Linac transport line were combined to achieve a good understanding of the transport line.

2. RF phase control.
Various correlations were measured to localize problem areas. A dedicated computer code was written to keep track of the drift in the different components. As a result of these investigations, temperature stabilization boxes were installed for the gun and linac low-level RF electronics. The daily phase drift was reduced by feed back correction from 30-50 degrees to approximately 10. The RF gun phase feedback program was finalized and is part of the ATF's routine operations

3. Mathcad tomography Software
The first version of the software was written in Visual C++. It comprised 1500 lines of code. The main disadvantage of that programming environment was having hidden physics under massive programming. We developed an ATF library that allows communicating between any Mathcad program and the ATF control database. The main advantage of this approach is the great visibility of the physics in the program. Following that, the Visual C++ version of the program was transcribed into the

Mathcad environment. The enhanced transparency of the program immediately elucidated a previously unseen problem. For example, a beam profile monitor image imperfection, such as the image of a fiducial mark, excites high frequency components in the filtered projections and causes a large numerical noise in the recovered phase space. Special digital filtering is under development.

4. Orbit correction

A special program was written to minimize steering effects from quadrupole magnets on beam line. Analysis of the collected data demonstrated that a re-survey of the quadrupoles is necessary to solve that problem. We plan to re-survey the quadrupole magnets on that line.

ACCOMPLISHMENTS:

1 post-docs supported.

Conference Proceedings:
M. Babzien, I. Ben-Zvi, R. Malone, X.-J. Wang, V.Yakimenko, Recent progress in emittance control of the photoelectron beam using transverse laser shape modulation and tomography technique, Proc. of the 1999 Particle Accelerator Conference, A. Luccio, W. MacKay, Editors, 2158, (1999)

LDRD FUNDING:

FY 1999	$201,393
FY 2000 (estimate)	$200,000

Attosecond Pulse Generation in High Harmonics

Louis F. DiMauro & Brian Sheehy 99-56

PROJECT DESCRIPTION:

The purpose of this project is the experimental characterization of the phase behavior of high order harmonics generated by an intense laser field, with the purpose of using harmonics to generate pulses on the attosecond time scale.

Recent advances in solid-state laser technology have permitted the generation of very intense short optical pulses. Near-infrared (~ 800 nm wavelength) pulses as short as 5 femtoseconds have been amplified to gigawatt power levels. Such pulses contain only a few optical cycles. A great many new physical phenomena have been revealed in this new dynamical regime, where optical fields can exceed atomic and molecular binding fields and pulse widths are on the time scale of molecular motion. One of these phenomena, High Harmonic Generation (HHG), the production of very high order harmonics of a laser driving field irradiating an atomic target, holds great promise as a coherent source of extreme ultraviolet (XUV) radiation. Harmonics as high as the 401st order, at a wavelength of 2 nm, have been produced. HHG may also open another new dynamical regime for study, through the possibility of creating attosecond pulses from the high harmonics. This would be the first coherent probe of matter on the time scale of electronic motion (for comparison, the period of the first Bohr orbit in hydrogen is 152 attoseconds).

Successful theoretical models of strong-field phenomena predict that phase nonlinearities of individual harmonics may be compensated to create pulses that are dramatically shorter than the driving laser's pulse width. Under some conditions the relative phases of a sequence of harmonics can also be "locked" and the harmonics combined to form even shorter pulses [1,2]. While many of the most exciting applications of attosecond pulses will be at the shorter XUV wavelengths produced by near-infrared laser systems, the experimental problem of measuring the phase behavior of pulses in the XUV is tremendous. Some sort of spectrally resolved autocorrelation is generally required, and both producing a suitable nonlinear interaction and making the optics required to accomplish this in the XUV would be extremely difficult, if not impossible. Such measurements may be achieved in the visible and ultraviolet though, and so we approach the problem by starting with a longer wavelength drive laser and generating harmonics in the visible and UV regions of the spectrum.

The ultrashort pulse mid-infrared laser system (Fig. 1) recently developed by us in the Chemistry department at BNL is unique in the world and ideally suited to this study. This system can produce intense pulses at wavelengths from 2.5-5.3 microns, at kilohertz repetition rates, with picosecond or femtosecond pulse widths, with easily varied phase behavior. We use this to irradiate alkali vapors and produce harmonics in the visible and UV spectrum. Making phase-sensitive measurements on these harmonics permits us to experimentally determine the steps required to compensate phase nonlinearities and produce ultrashort pulses. The compensation can then be accomplished both through the use of dispersive optics following harmonic generation and through adjustments of the phase behavior of the driving field.

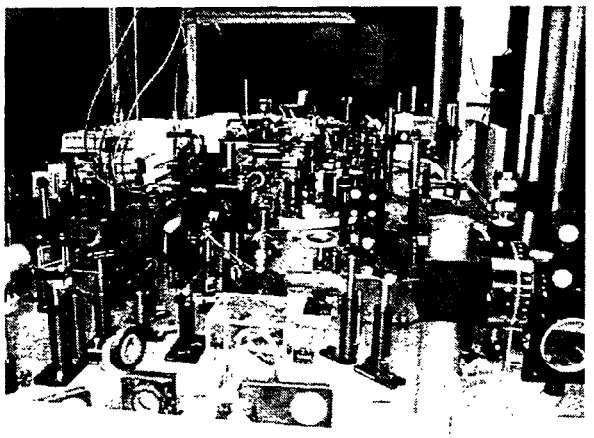


Figure 1. The ultrashort pulse kilohertz Mid-infrared laser developed in the BNL Chemistry Department.

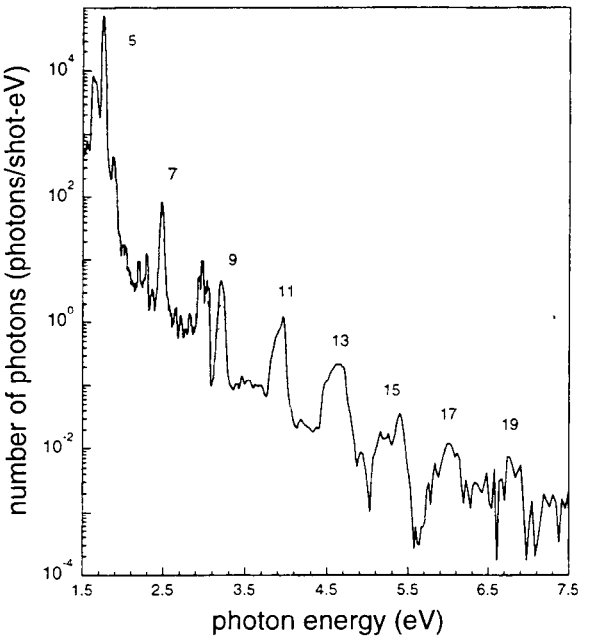


Figure 2. High harmonic spectrum generated by a 3.2 um, 1.9 picosecond light irradiating an atomic Rubidium vapor. The numbers indicate the harmonic order. Additional lines are due to atomic fluorescence.

TECHNICAL PROGRESS AND RESULTS – Fiscal Year 1999:

We have, in this fiscal year, accomplished all of our objectives for the production of sufficient harmonics to do phase-sensitive measurements and the construction of the apparatuses necessary to do these measurements.

Harmonic Production: A typical harmonic spectrum is shown in figure 2, displaying harmonics of 3.6 micron radiation generated in a Rubidium vapor. Harmonics are visible to the 19th order, or down to the UV cutoff of the apparatus. For the feasibility study prior to the beginning of this LDRD, we demonstrated harmonic production in a Potassium atomic beam. We have since surveyed harmonic production in the heavy alkalis (K, Rb, Cs). These studies were the first strong field experiments in this wavelength range, and important differences in the strong field physics at longer versus shorter wavelength were observed. These results are reported in references 3 and 4.

An atomic beam source is somewhat impractical in these studies, as the required target densities for efficient harmonic production are very high (1-30 torr). Beam ovens are quickly exhausted, and clogging and clouding of the chamber windows are problems. We have constructed a heat pipe oven source which provides a constantly recycled alkali vapor target. This source requires reloading only if the sample is changed or contaminated, clogging is eliminated, and clouding is greatly reduced. Using this source, loaded with Cesium, we are able to easily produce harmonics above the picojoule energy level.

Laser System: The behavior of the phase of the harmonics can be influenced by the behavior of the driving field, and for this reason extensive diagnostics are needed for the mid-infrared laser. We have constructed

an autocorrelator, using second harmonic generation in a potassium niobate crystal.

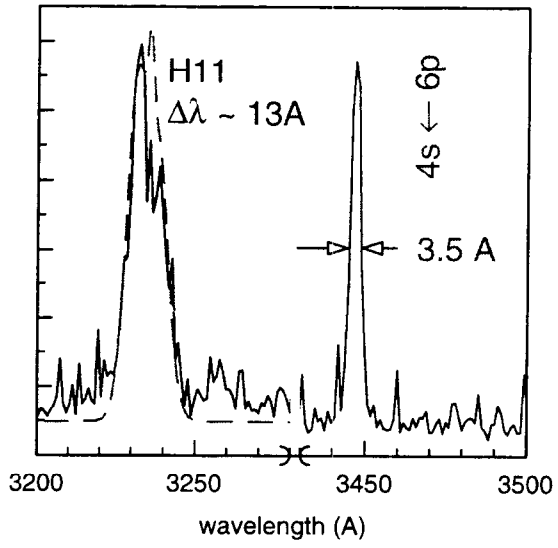


Figure 3. A typical measured (--) and calculated (--) harmonic line shape. The 11th harmonic of a 3.6 μm driving field irradiating Potassium. A nearby fluorescence line shows the resolution of the spectrometer.

By spectrally resolving this autocorrelation, a technique known as second harmonic generation frequency-resolved optical gating (SHG-FROG) [5] can be applied to obtain complete amplitude and phase information on the pulse. The spectrometer and scanning optics necessary for these measurements have already been incorporated in the working autocorrelator. A recently delivered linear detector array has only to be integrated into the system before this apparatus will be fully functional.

Spectral Measurements of the Harmonics: We have done extensive measurements of the yields and bandwidths of harmonics generated in the heavy alkalis. In figure 3 we show the measured spectral line shape of a harmonic in comparison with a theoretical model. The theoretical model [3] is based upon a calculation of the individual atomic response by numerically integrating the time dependent Schroedinger equation (TDSE)

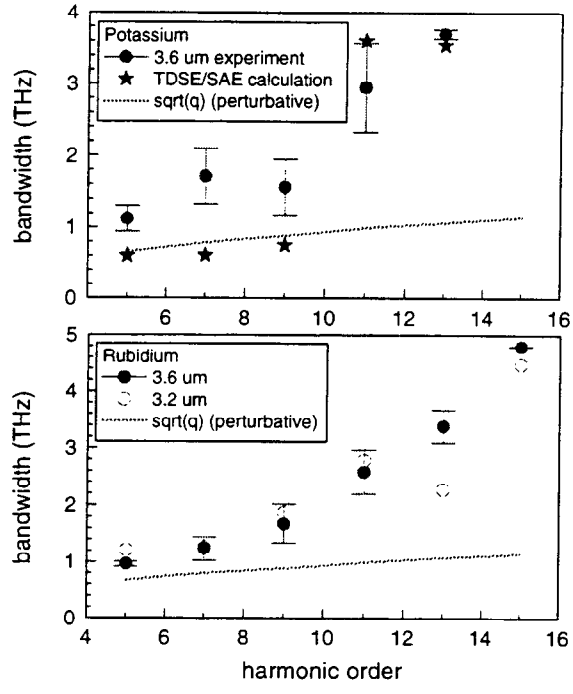


Figure 4. Harmonic bandwidth as a function of harmonic order. The possible pulse width is inversely proportional to the bandwidth. Note the large difference between the measurements and the perturbative value at large harmonic orders, indicating that a dramatic reduction in pulse width may be possible.

on a spatial grid, in the approximation that the field interacts primarily with a single active electron (SAE) moving in the average field of the other electrons. Both the amplitude and the phase of the atomic response are intensity-dependent, and so this response must be coherently summed over the intensity distribution of the laser focus. The agreement with theory is good in this as well as many other cases. In some circumstances though, lines shapes can show much more complex structure both in the theory and the experiment, and this behavior remains an open area of our investigations.

In Figure 4, measured bandwidths of harmonics generated in Potassium and

Rubidium are compiled as a function of harmonic order, and compared with our theoretical model and the bandwidth that one would expect from a purely perturbative harmonic generation process (i.e. a process in which the harmonic generation scales as I^q, where I is the driving field intensity and q is the harmonic order). While the theoretical model underestimates the bandwidth at lower harmonic order, the increase above the ionization threshold (harmonic 11 and above) is clear. The broad bandwidths beyond the perturbative prediction indicate that dramatic pulse shortening is possible, dependent on the behavior of the phase.

Current Status: We have now shown that there is sufficient intensity in the harmonics for a nonlinear interaction, having successfully frequency doubled the third and fifth harmonics. The next step is to make a direct temporal measurement of the harmonics by autocorrelation. These experiments are currently underway and we expect to have results soon. The autocorrelator design is achromatic, using all reflective optics so that the broad frequency range of the harmonics will not be a problem. It has also been designed and constructed to permit the easy integration of a monochromator, which will permit us to proceed directly to the next step: making SHG-FROG measurements on the harmonics. These measurements will give us the maximum possible information on the harmonic pulse and allow us to begin experiments on manipulating the harmonics to yield shorter pulses.

SUMMARY:

We have made extensive measurements of the yields and spectral properties of high harmonics. These measurements alone have provided valuable insight into the physics of strong-field processes [3,4]. Harmonics have been frequency-doubled and direct measures of harmonic pulse widths are in progress. The extension to phase-sensitive measurements is already incorporated into the experimental design. We expect very soon to obtain the first measurements that completely characterize the light generated by strong field HHG, and use those measurements to shorten the harmonic pulse.

REFERENCES:

1. P. Antoine, A. L'Huillier, and M. Lewenstein, "Attosecond Pulse Trains Using High-Order Harmonics" *Physical Review Letters* **77,** 1234 (1996).

2. K. J. Schafer and K. C. Kulander "High Harmonic Generation from Ultrafast Pump Lasers" *Physical Review Letters* **78,** 638 (1997).

3. B. Sheehy, J. D. D. Martin, L. F. DiMauro, P. Agostini, K. J. Schafer, M. B. Gaarde, and K. C. Kulander, "High Harmonic Generation at Long Wavelengths," submitted to *Physical Review Letters.*

4. M. B. Gaarde, , K. J. Schafer, K. C. Kulander, B. Sheehy, Dalwoo Kim, and L. F. DiMauro. "Strong Species Dependence of High Order Photoelectron Production in Alkali Metal Atoms" submitted to *Physical Review Letters.*

5. K. W. DeLong, R. Trebino, J. Hunter, and W. E. White, "Frequency-Resolved Optical Gating with the Use of Second Harmonic Generation" *J. Opt. Soc. Am B* **11**, 2206 (1994). For a comprehensive review of this and other FROG techniques, see R. Trebino *et al,* "Measuring Ultrashort Laser Pulses in the Time-Frequency Domain Using Frequency-Resolved Optical Gating" *Rev. Sci. Inst.* **68**, 3277 (1997)

LDRD FUNDING:

FY 1999	$109,251
FY 2000 (estimate)	$ 80,000

Development of a 2-D Ion Imaging Detector for VUV-FEL Applications

M. White *99-57*
R. Rao
R. J. Beuhler

PROJECT DESCRIPTION:

Statement of Work: In this project, we propose to develop a two-dimensional (2-D) ion-imaging spectrometer for the study of surface reaction dynamics, which takes full advantage of the intensity and tunability of the proposed BNL DUV-FEL. Ion-imaging will be accomplished via velocity focussing which preserves the angular distribution of the desorbed products over a large collection solid angle as required for surface studies using a conventionally-sized substrate and a line ionization source such as the VUV-FEL. Development of the 2-D detector requires extensive modeling of the ion optics to minimize the effects of the extended source geometry, as well as software development for analysis and re-construction of the velocity-resolved, spatial distributions. Initial testing will be performed in the laboratory using coherent VUV radiation generated by non-linear, up-conversion of tunable UV/VIS light from nanosecond laser sources.

TECHNICAL PROGRESS AND RESULTS – Fiscal Year 1999:

Purpose: In this work, we propose to develop a 2-D ion-imaging detector for studying surface reaction dynamics based on resonant and non-resonant ionization using coherent vacuum ultraviolet radiation (VUV). Initially, we will use VUV radiation produced by laboratory-based harmonic generation techniques for which our group has extensive experience. Ultimately, the imaging detector and surface spectrometer are being developed to take advantage of the much more intense VUV radiation produced by the Free Electron Laser (FEL) now under construction at the BNL Source Development Laboratory. The use of coherent VUV radiation as the ionization source offers several advantages over more conventional "universal" electron-impact ionization methods including tunability, and for the FEL, sensitivity. Tunability allows the detection of molecules at photon energies sufficient for ionization but below that for other interfering products or background gases, as well as below the dissociative ionization thresholds which complicates product identification. Furthermore, both laser-based and FEL-generated coherent VUV radiation have sufficient peak powers for use in one-photon resonant, two-photon ionization (REMPI) schemes for many small molecules (e.g., H_2, CO, CO_2, N_2). Such REMPI schemes are molecule-specific, and in some cases quantum-state specific, with sensitivities as high as 10^6 molecules per cm^3 per quantum state. For the FEL, the peak intensities are projected to be large enough (6×10^{14} photons/pulse at 100 nm) to allow an ionization efficiency of 10% which is orders of magnitudes higher than electron impact ionization source.

Approach: The main issues for design of the ion optics are (1) both the FEL and laser VUV beams are line sources over which ionization can take place and (2) the products originate from a distended source, *i.e.*, the metal substrate. We will adapt a new ion lens design, which has been recently demonstrated on gas-phase targets to dramatically improve the velocity focussing of ion-imaging systems. The 2-D spatial distribution of the ions will be

captured by a MCP-phosphor detector coupled with a CCD camera for full visualization. Image analysis software will also be developed to back-transform the raw images into velocity-resolved, spatial images of the desorbing products. The prototype 2-D imaging detector will be incorporated into an existing surface photochemistry apparatus equipped with a windowless VUV laser source for testing and optimization.

Technical Progress and Results: We have made extensive use of the SIMION 6.0 ion optics code to evaluate lens designs for spatially imaging a distended ionization source. The original design was based on the recent work of Eppink and Parker (Rev. Sci. Instrum. **68**, 3477 (1997)) who showed that a simple modification to a three-element electrostatic lens could result in velocity vector focussing. The latter would allow for the use of larger ionization volumes without distorting the ion image. Extensions to surface applications using VUV line sources would require velocity focussing over a length of up to 1-3 cm along the VUV beam direction. Ion trajectory simulations show that the three-element, thin-lens design of Eppink and Parker has serious chromatic aberations for such large source geometries and additional elements are required. Specifically, we found that a four-element system using thick ("tube") elements resulted in soft-focussing fields that could be tailored to provide imaging with source lengths as large as 2 cm. The conceptual design is shown in Figure 1.

Ion trajectory simulations indicate excellent velocity focussing with lens voltages typical of time-of-flight spectrometers with moderate mass resolution ($\Delta m/m \leq 1\%$). Other design challenges involved the spatial constraints of a "real" spectrometer, which in our case requires placement of the crystal substrate very close to the ionization volume. In addition, the laboratory VUV ionization source uses a capillary light guide (insulator) which must also be located very near the ionization volume. The physical design that meets both the spatial and ion optics criteria is currently being installed in the surface spectrometer and initial testing is underway.

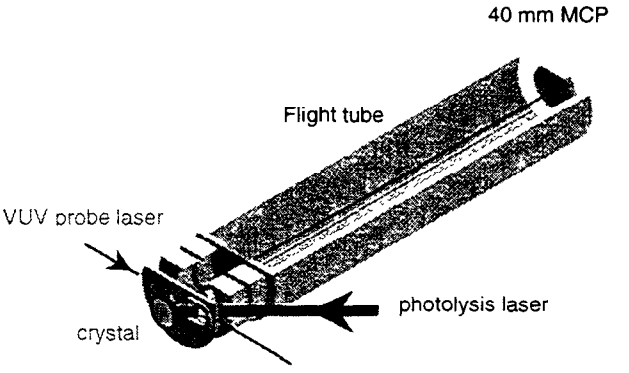


Figure 1: Schematic of ion-imaging time-of-flight detector.

ACCOMPLISHMENTS:

The work reported here was largely accomplished by a research associate (Dr. Raj Rao) who has considerable background in VUV ionization, surface science and particle detection. In addition, he has worked with CCD cameras and imaging systems in other contexts, i.e., dispersed fluorescence.

LDRD FUNDING:

FY 1999	$ 98,803
FY 2000 (estimate)	$ 80,000

Application of Quantitative MRI: Water Concentration and Blood-Brain-Barrier Permeability in Multiple Sclerosis

William D. Rooney *99-59*
Patricia Coyle
Lauren Krupp
Joanna Smiroldo
Charles Springer, Jr.
Frank Telang

PROJECT DESCRIPTION:

To develop and apply quantitative MRI techniques on BNL's 4 T scanner to better understand blood-brain barrier (BBB) function in health and disease.

The specific objectives are to determine if 1) brain water content is increased in multiple sclerosis (MS) white matter that appears normal on proton density MRI (so called "normal appearing white matter," NAWM) compared to control white matter, and 2) BBB permeability in MS NAWM is increased compared to healthy controls.

TECHNICAL PROGRESS AND RESULTS:

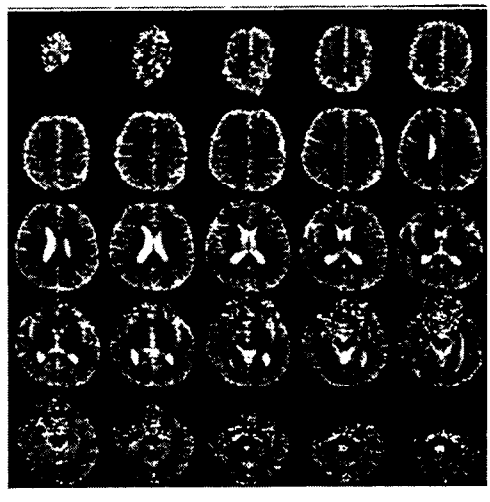
Progress has been made in several areas, most notably in the development of faster image acquisition methods, and initial measurements of BBB permeability in MS.

A. Fast 3D Quantitative T_1 Mapping: PURR-Dante Inversion Recovery Imaging

A major challenge in the development of quantitative T_1 techniques is to design a method that can collect data from the entire brain in a reasonable acquisition time using conventional magnetic resonance gradient hardware.

The MR literature is replete with fast imaging methods. However, most of these methods are demanding in terms of gradient performance. BURST is an ultrafast imaging technique that is much less demanding in terms of gradient performance. Here, we present an efficient method to provide full brain quantitative T_1 imaging by combining the concepts of Look-Locker (in the form of PURR) and 3D BURST-sampling techniques – a technique we call PURR-Dante.

The processed data set, T_1 maps for 25 axial slices, is shown below. In this experiment, the recovery was sampled at 32 (N_{TI}) non-linearly spaced inversion times (TI); 0.02 s $\leq$ TI $\leq$ 8 s and the total time to collect the (96x96x25)x32 complex points was 12.8 minutes. T_1 values for each brain volume element were extracted using a non-linear fitting routine. The image quality is high throughout most brain regions. ^1H_2O T_1 values extracted with this technique are in excellent agreement with values both from the standard PURR and conventional IR techniques. PURR-Dante data collection is twenty-five times faster than the standard PURR acquisition.

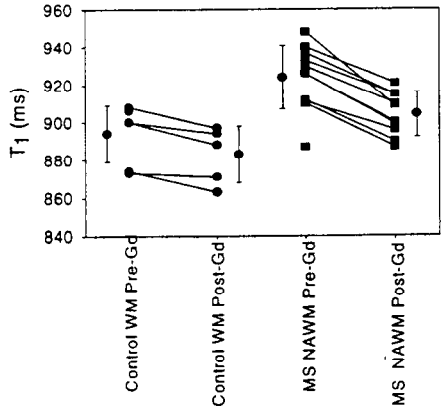


B. Initial measurements of brain water content and BBB permeability

Quantitative MRI techniques were used to measure brain ^1H_2O T_1 values in controls and MS subjects before and after administration of a gadolinium (Gd) contrast (re) agent (CR). Since ^1H_2O T_1 is decreased by interaction of water with the paramagnetic CR, and in a concentration dependent manner, the change in T_1 pre- and post-Gd can be used to measure to the concentration of CR in the brain.

Six healthy controls and twelve MS subjects were studied before CR administration. Quantitative T_1 data were obtained from five healthy controls and ten MS subjects before, and 20 minutes following, a 30 s intravenous injection of 0.1 mmol/kg CR. At least eight regions-of-interest, 20 mm^2 or greater, were selected from the centrum semiovale and periventricular white matter.

The data are plotted in the figure below. We find a highly significant 4% elevation in the water proton T_1 value of MS NAWM compared to control white matter ($P = 0.0017$) before administration of CR (i.e. pre-Gd). If we attribute this 4% increase in T_1 solely to increased water concentration, we estimate a 1.6% increase of the latter for MS NAWM.



The average T_1 value 20 minutes post-Gd was significantly reduced for the MS group. The mean paired difference in T_1, ΔT_{1Gd} [T_1 (pre-Gd) – T_1 (post-Gd)], was 10 (± 4) ms and 23 (± 7) ms, for the control and MS groups, respectively. The ΔT_{1Gd} was greater in MS NAWM compared to control WM ($P = 0.003$; Mann-Whitney). The most plausible explanation for increased ΔT_{1Gd} in MS NAWM is that the BBB is more permeable in MS NAWM than in white matter of healthy controls (i.e. more permeable to either water and/or CR). An alternate explanation is that regional blood volume is increased in MS NAWM. We are in the process of designing studies to distinguish between these possibilities.

SUMMARY:

During this funding year we have developed robust techniques that provide full-brain quantitative T_1 data in reasonable acquisition times. We have applied these techniques to better understand changes that occur in multiple sclerosis white matter that appears normal on conventional MRI scans. Our data suggests that, on average, water content is increased and BBB is more permeable in MS NAWM compared to control white matter.

ACCOMPLISHMENTS:

Collaborations

We have established two collaborations. The primary collaboration is with Drs. Patricia Coyle, Lauren Krupp, and Joann Smiroldo of the Department of Neurology SUNY/Stony Brook. The objective of this collaboration is to use quantitative MR techniques to improve understanding of pathology of MS. A second collaboration has been established with Drs. Truman Brown, Michael Ochs, and Radka Stoyanova of the Fox Chase Cancer Center.

The objective of this collaboration is to determine the utility of Principal Component Analysis and Bayseian techniques in improving the information content that can be extracted from brain water proton relaxographic imaging data sets.

Published Abstract

1. Fast 3D Quantitative T_1 Mapping – PURR-DANTE Inversion Recovery Imaging. William D. Rooney, Proc. Intl. Soc. Magn. Reson. Med. 1999; 7:10.

Manuscripts in preparation

1. Fast 3D Quantitative T_1 Mapping: PURR-Dante Inversion Recovery Imaging,
2. Quantitative Measurement of Blood-Brain Barrier Permeability in Multiple Sclerosis.

LDRD FUNDING:

FY 1999	$74,443
FY 2000 (estimate)	$75,000

In-Situ, Time-Resolved Studies of Catalysts for SO_X and NO_X Decomposition using Synchrotron Radiation

J.A. Rodriguez 99-62
J.Z. Larese

PROJECT DESCRIPTION:

Our project has three main objectives. The first one is to foster collaboration among members of the Catalysis (J.A. Rodriguez) and Materials (J.Z. Larese) groups in the Chemistry Department. The second one deals with the development of new and unique instrumentation for the characterization of catalytic materials under realistic industrial conditions. And the third one focuses on the use of this instrumentation to study the behavior of DeSOx and DeNOx metal/oxide catalysts that will have an important technological impact.

Instrumentation to characterize catalysts under industrial conditions at the NSLS. Catalysis plays a very important role in many processes used in the petrochemical and chemical industries. It is widely recognized that the development of techniques for the in-situ characterization of catalytic systems is one of the high priorities in the area of catalysis. Time-resolved x-ray diffraction and EXAFS can be used to characterize catalysts under the high pressure conditions of industrial processes. Experiments at X7B have established the feasibility of conducting sub-minute, time-resolved x-ray diffraction experiments under a wide variety of temperatures and pressure conditions (-190 ^{o} C < T < 900 ^{o}C; P 45 atm). One of the objectives of this project is to couple the instrumentation of X7B to an apparatus for the measurement of reaction kinetics at elevated pressures and temperatures. Post-doctoral fellows also will be working in the design and construction of reaction cells to perform time-resolved EXAFS experiments at X7B or X19. In this way, our Catalysis/Materials Science groups will be in possession of unique equipment for the characterization of heterogeneous catalysts.

SO_X and NO_X decomposition on magnesia and ceria based catalysts. The release of sulfur and nitric oxides (SO_X and NO_X) during the burning of fuels constitutes a major environmental problem. Due to an upgrade in the regulations for the control of environmental pollution, more efficient catalysts will be required for the removal or destruction of SO_X and NO_X compounds. Nowadays, millions of dollars are being spent in the search for these catalysts, and findings in this area can have a tremendous technological impact. It has been established that catalysts based on metal-promoted magnesium and cerium oxides can accomplish the decomposition of SO_X and NO_X molecules. However, it is not well understood how these promising systems interact with sulfur and nitric oxides, or how they operate at the elevated temperatures (400-800 K) and pressures (1-2 atm) used to carried out $DeSO_X$ and $DeNO_X$ processes.

TECHNICAL PROGRESS AND RESULTS- Fiscal Year 1999:

Approach: We have a lot of experience working with oxides and extensive knowledge on the surface chemistry of S-containing molecules. Our plan is to study the chemistry associated with DeSOx and DeNOx processes on oxides using techniques that are or will be available at the NSLS for surface and materials

characterization: from photoemission studies with model catalysts at U7A, to structural and high-pressure kinetic studies with "real-world" catalysts at X7B and X19. In addition, we plan to use a large array of techniques that are operational in our labs in the Chemistry Department (thermal desorption mass spectroscopy, infrared spectroscopy, scanning tunneling microscopy, etc). In this way, we will be able to get a complete picture of the problem, obtaining the basic knowledge that is necessary to fine tune and optimize the performance of catalysts and sorbents used in DeSOx and DeNOx operations.

Technical Progress and Results: In the present year we have examined the adsorption of SO_2 on CeO_2, ZnO and MgO. Details of the chemistry of the molecule on the oxide surfaces are presented below. Our results have shown that a combination of photoemission and XANES is a very powerful approach for investigating these systems. Progress has been made in the design of a cell for in-situ studies with EXAFS. This instrument should become operational within the next year.

Interaction of SO_2 with CeO_2 and model Cu/CeO_2 Catalysts. CeO_2 and Cu/CeO_2 are effective catalysts/sorbents for the removal or destruction of SO_2. Synchrotron-based high-resolution photoemission, XANES, and temperature programmed desorption were employed to study the reaction of SO_2 with pure and reduced CeO_2 powders, ceria films (CeO_2, CeO_{2-x}, Ce_2O_{3+x}) and model Cu/CeO_2 catalysts. The results of XANES and photoemission provide clear evidence that SO_4 was formed upon the adsorption of SO_2 on pure powders or films of CeO_2 at 300 K. The sulfate decomposed in the 390-670 K temperature range with mainly SO_2 and some SO_3 evolving into gas phase. At 670 K, there was still a significant amount of SO_4 present on the CeO_2 substrates. The introduction of O vacancies in the CeO_2 powders or films favored the formation of SO_3 instead of SO_4. Ceria was able to fully dissociate SO_2 to atomic S only if Ce atoms with a low oxidation state were available in the system. When Cu atoms were added to CeO_2 new active sites for the destruction of SO_2 were created improving the catalytic activity of the system. The surface chemistry of SO_2 on the Cu-promoted CeO_2 was much richer than on pure CeO_2. These results help to explain the behavior of ceria in several catalytic processes: oxidation of SO_2 by O_2, reduction of SO_2 by CO, automobile exhaust converters.

Reaction of SO_2 with ZnO(0001)-O and ZnO Powders: Synchrotron-based high-resolution photoemission and XANES were used to study the interaction of SO_2 with ZnO(0001)-O and polycrystalline films and bulk powders of ZnO. The adsorption of SO_2 on the (0001) O-terminated face of ZnO at 110 K produced SO_3 species which were stable up to temperatures well above 400 K. On polycrystalline ZnO, the $Zn \leftrightarrow SO_2$ interactions were very weak, there was no decomposition of the admolecule, and evidence for bonding of Zn to SO_2 was found only at low temperatures (~ 100 K) when the adsorbate had a limited mobility on the surface. At 300 K and moderate pressures, SO_2 only reacted with the O centers of ZnO forming mainly SO_3 groups. Part of the formed SO_3 decomposed at temperatures between 400 and 600 K with evolution of SO_2 into gas phase ($ZnSO_{3,solid} \Rightarrow SO_{2,gas} + ZnO_{solid}$). At 600 K, a significant amount of SO_3 was still present on the ZnO systems. Reaction with O_2 led to a $SO_3 \Rightarrow SO_4$ transformation on ZnO(0001)-O and powders of ZnO previously exposed to SO_2. SO_4 was directly formed during the

adsorption of SO_2 on polycrystalline surfaces of zinc oxide that were rich in O atoms which had a low coordination number (< 3) and a relatively high mobility. On ZnO(0001)-O and polycrystalline ZnO, there was no decomposition of sulfur dioxide. Promotion with K and Cs facilitated the cleavage of S-O bonds. After dosing SO_2 to ($\sqrt{3}$ x $\sqrt{3}$)-K/ZnO(0001)-O and ($\sqrt{3}$ x $\sqrt{3}$)-Cs/ZnO(0001)-O at 300 K, several sulfur species (S, SO_3, SO_4) coexisted on the alkali promoted surfaces whereas only SO_3 was formed on the pure ZnO(0001)-O system.

Reaction of SO_2 with MgO(100) and MgO powders Photoemission, XANES, temperature programmed desorption, and x-ray diffraction were used to investigate the adsorption of sulfur dioxide on MgO(100) and powders of MgO. At 100 K, the chemisorption of SO_2 on MgO(100) produces mainly SO_3 and a minor amount (~ 10 % at saturation coverage) of SO_4. Heating from 100 to 300 K induces a partial $SO_3 \Rightarrow SO_4$ transformation, as a consequence of the reaction of SO_3 with the O sites of the MgO(100) surface. Additional heating to 500 K further increases the SO_4/SO_3 ratio on the surface, but the total amount of adsorbed sulfur species decreases due to the desorption of SO_2. At 600 K, there are no SO_x species and only a small amount (< 0.05 ML) of atomic sulfur is left on the oxide surface. Similar trends are found after depositing SO_2 on bulk powders of MgO at room temperature and subsequent heating to 625 K. OH groups chemisorbed on MgO(100) or MgO powders favor the formation of SO_4 at the expense of SO_3. A $SO_3 \Rightarrow SO_4$ transformation is observed after exposing SO_2/MgO systems to a stream of O_2/He at 380-430 K.

ACCOMPLISHMENTS:

Three articles have been submitted for publication (two of them are already accepted):

"Interaction of SO_2 with CeO_2 and Cu/CeO_2 Catalysts: Photoemission, XANES and TPD Studies," J.A. Rodriguez, T. Jirsak, A. Freitag, J.C. Hanson, J.Z. Larese and S. Chaturvedi, Catal. Lett. in press.

"Reaction of SO_2 with ZnO(0001)-O and ZnO Powders: Photoemission and XANES Studies on the Formation of SO_3 and SO_4," J.A. Rodriguez, T. Jirsak, S. Chaturvedi, and M. Kuhn, Surf. Sci. in press.

"Chemistry of SO_2 on Model Metal and Oxide Catalysts: Photoemission and XANES Studies," J.A. Rodriguez, T. Jirsak, S. Chaturvedi, J. Hrbek, A. Freitag, and J.Z. Larese, Stud. Surf. Sci. Catal. submitted.

Results have been gathered for at least another two articles. A review of these studies will be presented at the 12th International Congress of Catalysis.

Funds from this LDRD provided support for two postdoctoral fellows during this fiscal year and similar support will be necessary in the next two years to fully achieve the objectives of the project.

LDRD FUNDING:

FY 1999	$121,957
FY 2000 (estimate)	$ 50,000

Advance Object Oriented Databases On Linux Systems

David Stampf *99-63A*

PROJECT DESCRIPTION:

This project was to determine the feasibility of running a very high function commercial Object Oriented Database Management System under Linux, which is an Intel processor compatible open source operating system.

APPROACH:

A widely used commercial OO Database Management System, Objectivity, was selected for this project based on its use in various DOE funded projects some of which anticipated extensive use of the Linux operating system. An agreement was reached with the company to collaborate in the process of porting the software to the Linux system and for initial testing of the result by various interested user communities.

TECHNICAL PROGRESS AND RESULTS:

A BNL staff member performed the port of the OODBMS code to the Intel/Linux operating system at the Objectivity site with the help of Objectivity personnel. The resultant libraries were then made available to BNL, SLAC and CERN for testing and evaluation. After an additional iteration of the porting process based on a more up-to-date version of the Operating System and the C compiler, a version was established that the users groups found to be fully functional.

SPECIFIC ACCOMPLISHMENT:

Based on this demonstration Objectivity has made Linux one of the standard operating systems on which they support their DBMS. They have a fully supported product, which is being widely used both at the sites named above and by other Objectivity customers. This permits use of a very cost effective commodity/Open Source platform to run a high functionality commercial database.

LDRD FUNDING:

FY 1999 $114,685

Mobile Agent Based Monitoring of Distributed Computing Systems

Richard Ibbotson *99-63B*

PROJECT DESCRIPTION:

The goal of this project is to demonstrate the feasibility of using Java based mobile agents, a new software technology, to produce a platform independent, highly flexible tool set capable of measuring end-to-end performance for distributed computing systems in a wide variety of metrics.

APPROACH:

A Java mobile agent system will be selected and used to develop a template for a computing facility performance-measuring instrument. An overall clearing house for instruments and their reports will be established and the feasibility of using agents as instruments demonstrated by instantiating and operating one or more such instruments.

TECHNICAL PROGRESS AND RESULTS:

A particular implementation of Java mobile agent technology, IBM Aglets, was selected for conducting this demonstration. The available agent mobility patterns were investigated, and a framework for dispatching agents and receiving and storing their reports developed. In the coming year a display system will be added to the report store, a template for instruments based on these agents will be developed and one or more functional instruments implemented and demonstrated.

SPECIFIC ACCOMPLISHMENTS:

The project has not yet reached the point of verifying the feasibility of this approach.

LDRD FUNDING:

FY 1999	$180,000

Demonstration of Advanced Commercial Ethernet Technology

Terence Healey *99-63C*

PROJECT DESCRIPTION:

The goal of this project is to demonstrate the feasibility of implementing very high performance LANs based on commercial next generation Ethernet products. The issues are: Is a complete set of such products available? Are they reliable and robust enough for production use? Do they interoperate with each other properly? What levels of functionality and performance do they supply?

APPROACH:

Contrary to predictions four years ago that Asynchronous Transfer Mode (ATM) technology would dominate the future of Local Area Network (LAN) evolution, a variety of innovations to the Ethernet standard have appeared and now seem destined to play a significant role in the LAN market for the foreseeable future. While of modest and continuously decreasing cost, advanced commercial Ethernet products seem to offer performance comparable to very high performance network options including ATM and HIPPI, both of which are very much more costly. A set of products was to be identified and acquired via loan or purchase. This set would then be integrated into one or more systems and tested for interoperability, functionality, performance, and reliability.

TECHNICAL PROGRESS AND RESULTS:

The following advanced Ethernet technologies were identified as being part of a complete high performance set; Gigabit, 10 Gigabit, Jumbo Frame, physical line trunking and the use of VLANs.

Commercial vendors were identified for most of these products and Jumbo frame capable Gigabit Ethernet switches and Network Interface Cards from ALTEON were acquired and tested. Initial tests indicate that Gigabit Ethernet in simple applications works very well, Jumbo frame Gigabit Ethernet works on Sun systems but some interoperability problems have been encountered in working with heterogeneous distributed systems including IBM/AIX, Intel/Linux, and Sun/Solaris. Different problems have been encountered trying to interoperate ALTEON hardware with other Gigabit capable switches such as those from Packet Engines. Tests of VLANs, physics trunking of Gigabit lines, 10 Gigabit Ethernet, and Gigabit capable network sniffers remain to be completed.

SPECIFIC ACCOMPLISHMENTS:

Tests performed to date indicate that simple Gigabit Ethernet technology is mature enough for production use. However, interoperability problems do exist with Jumbo frame Gigabit Ethernet, though vendors seem anxious to pursue and correct them. The investigation of more complex functionality and other components of a complete LAN system remain to be completed.

LDRD FUNDING:

FY 1999	$180,000

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

2000 PROPOSED PROGRAM*

*New projects authorized for funding as of October 1, 1999.

(00-05A) Exploration of the Object Oriented Approach to Reconstruction Algorithms
Howard Gordon (FY2000 Funding $100,000)

The objective of this project is to explore the resources required to design and implement this code in a fully modern Object Oriented method. This work will be the basis for determining the feasibility of improving the allocation of resources needed to develop the major analysis software for future high energy physics experiments.

(00-05B) Assessment of GEANT4 as a Model for the ATLAS Liquid Argon Calorimeter Test Beam Data - Howard Gordon (FY 2000 Funding $100,000)

The goal of this project is to explore the feasibility of GEANT4 as a Model for the ATLAS Liquid Argon Calorimeter Test Beam Data. GEANT4 is a new software simulation package developed by a world wide collaboration. It is based on the very successful GEANT3 package, which was developed at CERN in Geneva, Switzerland. It has been implemented in a fully Object Oriented framework but has not been fully tested. The concept is to compare results for energy and position resolution from GEANT4 to actual ATLAS test beam data. If successful, this will allow us to plan the amount of resources needed to do this for all aspects of the ATLAS detector.

(00-06) Probing Extreme QCD: Articulating the Physics Goals of an Electron-Relativistic Heavy Ion Collider (eRHIC) at BNL (FY 2000 Funding $85,000)
R. Venugopalan

An electron-relativistic heavy ion collider (eRHIC) can probe a novel, highly non-linear, regime of high parton densities in QCD at small values of Bjorken x and Q^2 on the order of several GeV^2. Comparable parton densities at an electron-proton (ep) collider would requires x's that are three to five orders of magnitude smaller. Further, an eA collider provides a unique opportunity to investigate the space-time structure of scattering in QCD-various striking phenomena arise from QCD coherence at small x. We propose to address concretely the physics goals of a future electron-relativistic heavy ion collider. In particular, we would like to quantify the energies, luminosities, and detector requirements that would be necessary to measure, with a high level of precision, the various experimental signatures of non-linear QCD.

(00-25) Novel Techniques To Measure Aerosols And Aerosol Precursors
S. Schwartz (FY 2000 Funding $150,000)

Tropospheric aerosols are important environmental agents, impacting climate, human health, etc. Concern over these effects and the need for understanding of aerosol processes needed to develop strategies to meet prospective air quality standards suggest that there will be substantial new research efforts addressing tropospheric aerosols in DOE and other agencies in the next several years. This project is to investigate and demonstrate novel techniques to measure aerosol composition and properties. This project consists of two activities. First, rapid, real-time measurement of aerosol chemical composition. Traditionally aerosols are collected on filters and analyzed subsequently by wet chemical techniques. This approach suffers from low time resolution (limiting aircraft applications) and from the fact that the data are available to investigators weeks after the data are taken. Second,

multiple-humidity tandem differential mobility analyzer (TDMA). Response of aerosols to relative humidity is an aerosol important property that must be characterized. A multiple-humidity TDMA has been designed based on a novel concept which permits the sampling and separation of aerosols simultaneously into three different packets so that changes in relative humidity can be imposed and the growth observed.

(00-27) Nanocomposites of Silicon Polymorphs and Related Semiconductor Systems
D. O. Welch (FY 2000 Funding $80,000)

We propose to use methods of high-resolution transmission electron microscopy (TEM) and theoretical analysis to understand the mechanisms of formation and properties of nanocrystalline dispersions of metastable high-pressure polymorphic phases of Si in normal diamond-cubic Si matrices, as well as to investigate related shock-synthesized nanocomposites based on other diamond-structure semiconductors. This novel material, recently developed at SUNY-SB, presents excellent opportunities for scientific studies of basic materials science with significant implications for energy-related applications such as opto-electronics.

(00-32) Microvascular Endothelial Cells as Targets for Ionizing Radiation: In Vitro and In Vivo Models (FY 2000 Funding $100,000)
L. Pena

A new emphasis on the radiobiology of endothelial cells is proposed which utilizes an in vivo model (rat brain) and in vitro models (2D endothelial cell culture and 3D endothelial/astrocyted co-culture). This coincides with research currently underway in our laboratory group. The goals are to modify the radiation sensitivity of these cells by genetic and pharmacological manipulation of the lipid second messenger ceramide signal transduction pathway via the SAPK/JNK cascade. One radio-protectant we are currently studying, bFGF, will be applied in the in vivo model in an attempt to prevent late effect injury mediated by endothelial cell damage, and will also be utilized in the in vivo models. This proposed project makes use of the unique scientific resources of the BNL Medical Department, NSLS, and AGS.

(00-35) Investigating Surface Chemical Reactions and Kinetics from the Atomic to the Nano Scale (FY 2000 Funding $50,000)
J. Hrbek

In this project, we propose to use our Variable Temperature Scanning Probe Microscope (VT SPM) to study several surface reactions and phenomena closely related to catalysis and as a bridge to a more expanded effort in nanoscience, including the eventual addition of another FTE who is expert in SPM techniques. Furthermore, we wish to extend the capability of this instrument by investigating the feasibility of creating in effect a Chemical Force Microscope. The new device would be created by depositing controlled amounts of sulfur, carbon, clusters of transition metals and other related materials onto an AFM tip and then using the modified tip as a probe for identifying chemically active sites on a variety of materials by scanning it in the conventional manner.

(00-40) The Structure of Membrane Proteins: Monolayers and Thin Films
B. Ocko (FY 2000 Funding $65,000)

The goal of this project is to provide insight into the structure of membrane proteins using surface x-ray scattering techniques. These techniques: grazing incident angle diffraction and x-ray reflectivity, have been successfully applied to a wide variety of physics and materials problems and are particularly applicable in these biological systems where other structural techniques are limited. Nearly a third of all proteins cannot be readily crystallized. As a result, conventional x-ray diffraction techniques have contributed little to our structural understanding. By using well-defined interfaces (i.e. the water/air interface), it is possible to orient biological thin films and interfaces and to obtain detailed molecular information, albeit at resolutions coarse on the atomic scale. These techniques offer considerable advantage over conventional powder diffraction techniques carried out on unaligned samples.

(00-42A) Mobile Agent Based Monitoring of Distributed Computing Systems
R. Ibbotson (FY 2000 Funding $150,000)

The goal of this project is to prove the concept of using Java based mobile agents, a new innovative technology, to produce highly flexible, platform-independent, tool sets capable of measuring end-to-end performance in a wide variety of metrics.

(00-42B) Demonstration of Advanced Commercial Ethernet Technology
T. Healy (FY 2000 Funding $100,000)

Contrary to predictions four years ago that Asynchronous Transfer Mode (ATM) technology would dominate the future of Local Area Network (LAN) evolution, a variety of innovations to the Ethernet standard have appeared and now seem destined to occupy a significant if not dominate role in the LAN market for the foreseeable future. The goal of this project is to establish that a complete set of next generation commercial Ethernet components exists and that they are mature enough to make it feasible to produce a production system based on them. This shall be accomplished by beta testing, for performance, reliability, and manageability, several of these technological innovations in a realistic test bed environment and determining how they interact with each other. The innovative Ethernet technologies to be tested include Gigabit, 10 Gigabit, Jumbo Frame, physical line trunking and the use of VLANs.

(00-42C) Cyber Security for Wide Area Distributed Collaborations
S. Misawa (FY 2000 Funding $100,000)

The conflict between cyber security concerns and the access needs of wide area distributed collaborations pose a major problem of particular importance to the current and next generation of large High Energy and Nuclear Physics experiments. The goal of this project is to establish the feasibility of an adiabatic approach to supplying adequate cyber security without extensive disruption to the use of computing facilities by such user communities. The demonstration architecture includes ssh gateways, application proxies, substantial host service restriction and monitoring and the use of a firewall to monitor and control overall access.

(00-42D) Data Mining Strategies for HENP Experiments
B. Gibbard (FY 2000 Funding $100,000)

High Energy & Nuclear Physics experiments today require specialized data mining to make effective use of physicists' time and the available data. There can be dramatic differences in the amount of sophistication and effort that go into the systems that support this data mining. The goal of this project is to study the feasibility of using simple data mining strategies in place of more sophisticated approaches. It is important to understand if there are regimes in which simpler and less expensive strategies can produce comparable or perhaps even superior performance to heavier weight systems. Two different strategies have been proposed with the goal of extracting selected data subsets from Petabyte scale data sets located on tertiary storage. One involves the correlation of relatively complex data queries at the object container level and has been under development for the past three years. The second involves the correlation of simple file level requests.

(00-42E) Parallel Linux Systems
T. Throwe (FY 2000 Funding $100,000)

The goal of this project is to investigate an innovative concept system for performing parallel system administration in a manner that scales well with the number of computers and allows for customization based on hardware configuration and individual problem type. The approach is to initially *clone* a prototype computer's operating system image across the Local Area Network in each member of an array of computers. Each computer then uses a set of database-maintained scripts to customize its own operating system image before doing a final reboot to its working operating system.

(00-43) Understanding the Pathways of Obiquitin Dependent Proteolysis
M. Bewley (FY 2000 Funding $266,000)

The overall goal of this proposed project is to understand the structural basis for substrate targeting by the ubiquitin system and in particular the targeting of substrates that are involved in cell cycle control. This process appears to be combinatorial in nature and at present, the reliability computer-based strategies for correctly predicting protein-protein interactions is limited, at best. Therefore, it will be important to characterize a variety of complexes to better understand the rules that govern their formation. This approach may ultimately lead to the development of better prediction methods.

(00-45) New Protein Expression Tools for Proteomics
P. I. Freimuth (FY 2000 Funding $45,000)

A critical phase of the Proteome lab initiative is the production of highly purified, biologically active proteins in quantities that are suitable for crystallization and x-ray diffraction. Although the T7-based system for protein overexpression in bacteria that was developed at BNL often performs well, there are many cases where the proteins overexpressed in this system are unable to adopt their native conformations and aggregate as mis-folded proteins within the bacterial cells. Specifically, the expression of many cytosolic proteins and almost all membrane-associated proteins derived from eukaryotic organisms is problematic in the T7 system. The major reason for this failure is that bacterial cells lack the specialized molecular machines that catalyze protein folding and modification

in eukaryotic cells. This is a proposal to develop new tools for expression of both of these problematic classes of proteins, and is based on results of our earlier studies.

(00-47) High-Throughput Structure Determination for the Human Proteome Project
W. Studier (FY 2000 Funding $600,000)

As the Human Genome Project nears its goal of elucidating the complete instruction set for human life, attention is turning to the proteins specified by that genome. The biochemical reactions necessary for life are carried out primarily by proteins, and learning the functions of the approximately 100,000 proteins specified by the human genome is a great challenge and opportunity. A Human Proteome Project, a systematic effort to learn the roles and functions of RNAs and proteins, is a natural extension of the Human Genome Project, capitalizing on the investments already made. It would have an impact at least as great as the Human Genome Project in promoting an understanding of biological systems and stimulating scientific and commercial activity.

(00-49) Design Study of a Solid Rod Target for Spallation Neutron Source
J. Hastings (FY 2000 Funding $300,000)

This project is to investigate the feasibility of a dedicated facility at the AGS capable of investigating all aspects of the SNS production. This project is for the design, construction and beam testing of a solid rod target optimized for the AGS facility. The work will specifically address the mechanical issues and transient behavior to provide a long lifetime design, which is passively safe with a failure of the cooling loop. The proton beam extraction and transport needed for the tests of the prototype target will be designed and constructed. A full testing program will be carried out to verify the design concept.

(00-61) Remote Full-Field Dynamic Optical Measurement of Structural Integrity
R. Hall (FY 2000 Funding $58,000)

The goal of this research is to explore the feasibility of using a remote, non-contact sensor system capable of continuously monitoring and evaluating the conditions of complex structures under real life fatigue and corrosion. This research will lead to a full-scale proof of principle demonstration of this innovative concept on a structure on the Lab site. If successful, this work can lead to enhanced public safety, reduced traffic congestion, and support DOE's programs on smart buildings and industries of the future.

(00-93) Muon Collider and Storage Ring Neutrino Beam Study
R. Palmer (FY 2000 Funding $200,000)

The goal of this project is to perform a preliminary technical analysis and feasibility study of a muon storage ring at Brookhaven. The high-energy muon storage ring could serve as a source of intense neutrino beams. The research shall identify areas of major uncertainty, crucial design issues, and topics requiring further theoretical or experimental investigation.